intellegens

Challenges & opportunities of adopting AI in materials design

Current applications & future directions

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AI in materials design

Challenges

Opportunities

Real world

AI FOR MATERIALS DESIGN - THE PROMISE?

Discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost

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Quick poll: Who in the room has tried to use AI to solve a current problem - and out of those - were any of them successful?

1. CHALLENGES

Industry

Understanding of applicability
Conservative
Validation
Providers / education
Digitalisation
    Priority, integration

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    New experiments & simulations
Security
Storage aggregation

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Budget & investment

Waste time & effort
Grant funding
Innovation
    Invest time and money but fails
    or do not invest and fall behind
Intellectual property

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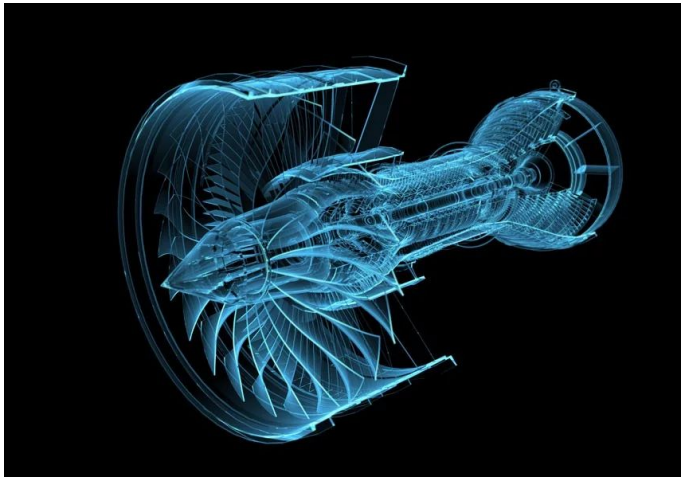
Question

What other challenges in adoption have you encountered and which of these is the biggest barrier?

2. DISCOVERING A NEW ALLOY FOR ROLLS ROYCE



Problem

Commercially available alloys do not have the optimal balance of properties required for specific engineering applications

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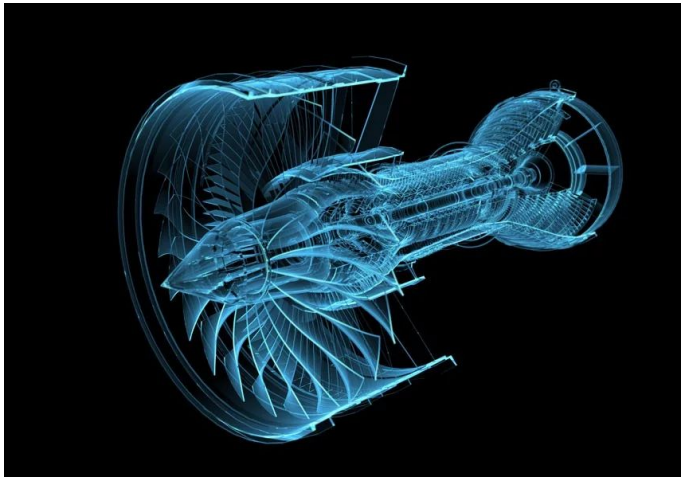

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Applied novel neural network to combine sparse experimental data with computational thermodynamic predictions to design a new alloy

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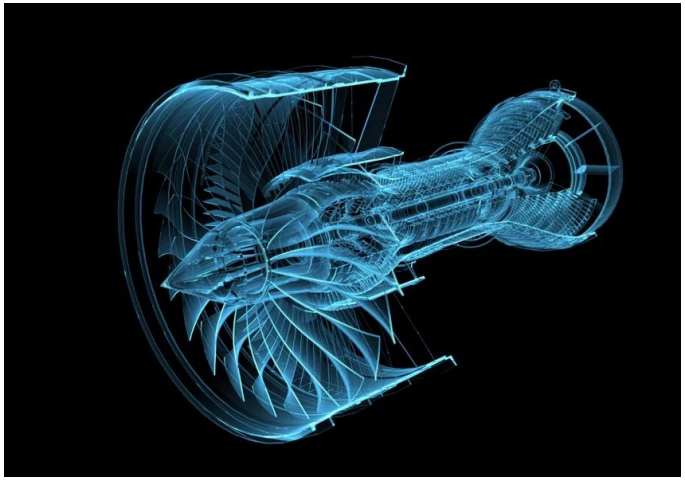

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Applied novel neural network to combine sparse experimental data with computational thermodynamic predictions to design a new alloy

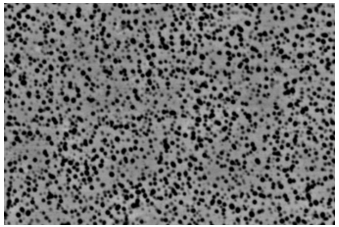
Outcome

Designed a nickel-base superalloy alloy that fulfills 11 different physical criteria

Experimentally verified and patented

2. OPPORTUNITIES AND APPLICATIONS

3D printing alloy



VARIABLES

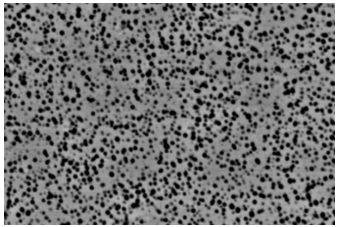
Composition
Printing procedure
Processing

TARGETS

Strength
Oxidation
Cracks

2. OPPORTUNITIES AND APPLICATIONS

3D printing alloy



Batteries

VARIABLES

Composition
Printing procedure
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Chemistry
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Geometry

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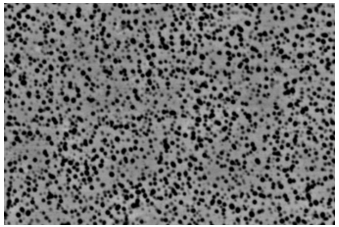
Cracks

Charge capacity
Charging time
Lightweight

2. OPPORTUNITIES AND APPLICATIONS

3D printing alloy



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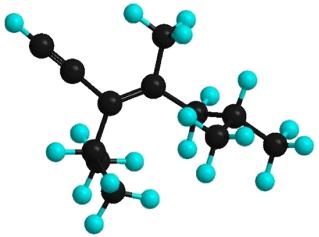
Lubricants



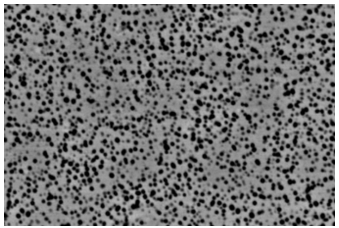
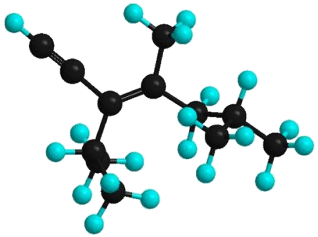
VARIABLES

Branches
Functional groups
Additives

TARGETS

Viscosity
Flash point
Pour point

2. OPPORTUNITIES AND APPLICATIONS

	3D printing alloy	Batteries	Lubricants	Drug design
				
VARIABLES	Composition Printing procedure Processing	Chemistry Processing Geometry	Branches Functional groups Additives	Chemistry Solute Dosage
TARGETS	Strength Oxidation Cracks	Charge capacity Charging time Lightweight	Viscosity Flash point Pour point	Activity Toxicity Side effects

Do you see any **current opportunities** that AI could help with?

3. REAL-WORLD SOLUTIONS

Our collaborations have used data to deliver

Maximised formula performance for multiple target properties

Reduced prototype costs - reduction in experiments

Reduced material costs - minimization of expensive properties

Reduced environmental impact

Standardised design process across a company

3. REAL-WORLD: CHROMIUM IN STEEL

Advantages Chromium makes steel corrosion resistant and hard

Disadvantages Chromium is toxic, environmentally unfriendly, and expensive

Challenge Design a new steel with same physical properties but less Chromium

Current heuristic approach Industry experts, duplicate historic mixes

Solution Tool to run “virtual experiments” to simulate low-chromium steels, whilst maintaining physical targets

3. REAL-WORLD: CONCRETE FOR CONSTRUCTION

Challenge Deliver best mix based on project conditions

380 factors Local sand, local aggregate, cement, environmental conditions, project type, travel time, target strength, admixtures

Current approach Industry experts, pick from historic mixes / similar projects

Solution Tool to suggest optimal “mixes” considering cost, location, and time of year
Knowledge from previous projects shared and adding future value

What **tools** do you see in the future
that can accelerate materials design?

CONTACT

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