Intellegens

Materials discovery with artificial intelligence

Gareth Conduit

Neural network algorithm to

Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

Accelerate materials and drugs discovery

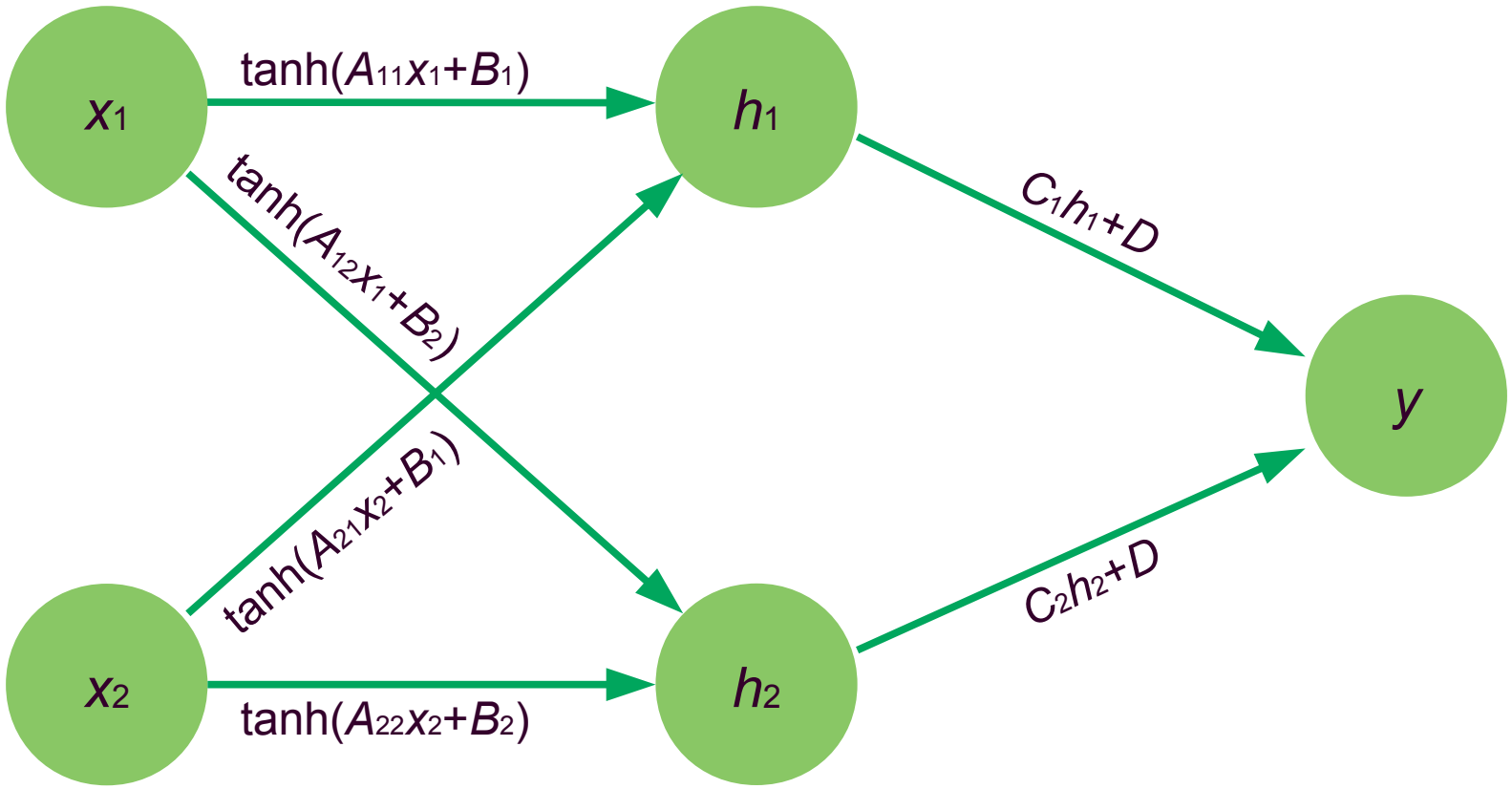
Generic with **proven** applications in materials discovery and drug design

Neural network: a black box

Neural network: train on complete data

Neural network: train on complete data

Neural networks: architecture

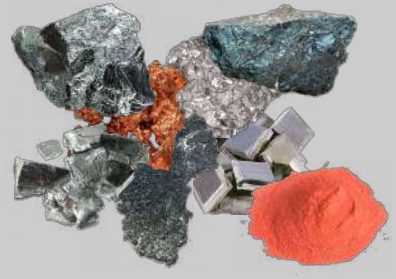


Neural network trains on fragmented data

Neural network predicts on fragmented data

Black box for materials design

Composition



Properties

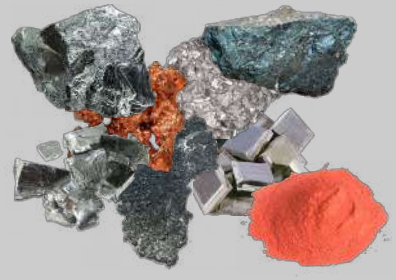
UTS

Hardness

Cost

Training the neural network

Composition



Properties

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Hardness

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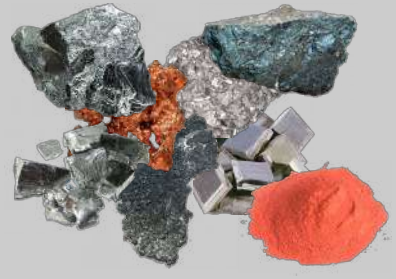
Neural network for materials design

Composition



Properties

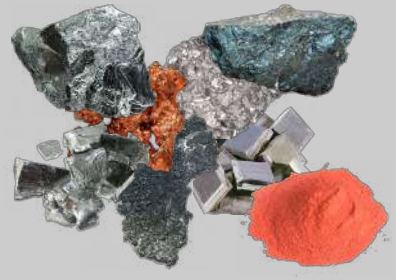
UTS

Hardness

Cost

Neural network that can exploit all correlations

Composition



Properties

UTS

Hardness

Cost

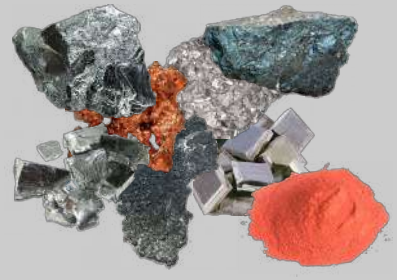
Simulations

Density Functional

Molecular dynamics

Finite element

Composition



Properties

UTS

Hardness

Cost

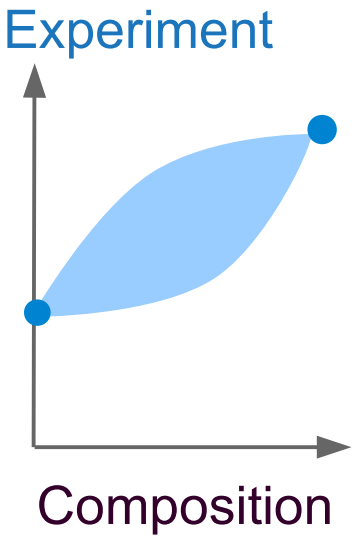
Simulations

Density Functional

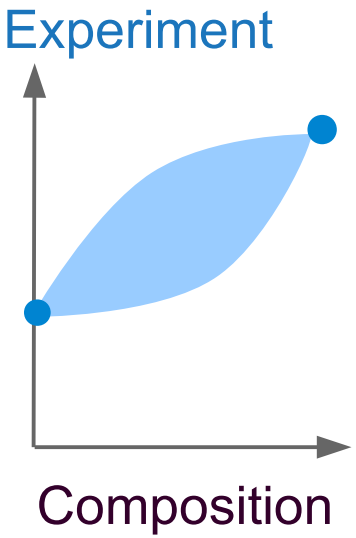
Molecular dynamics

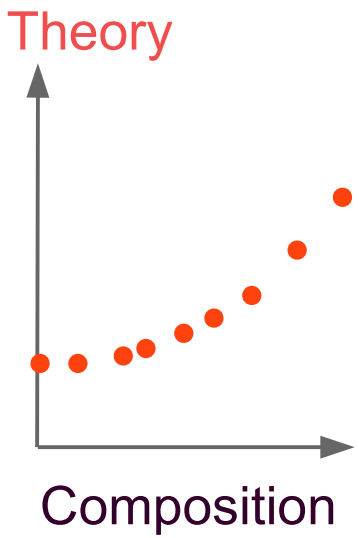
Finite element

Neural network trained on experimental data

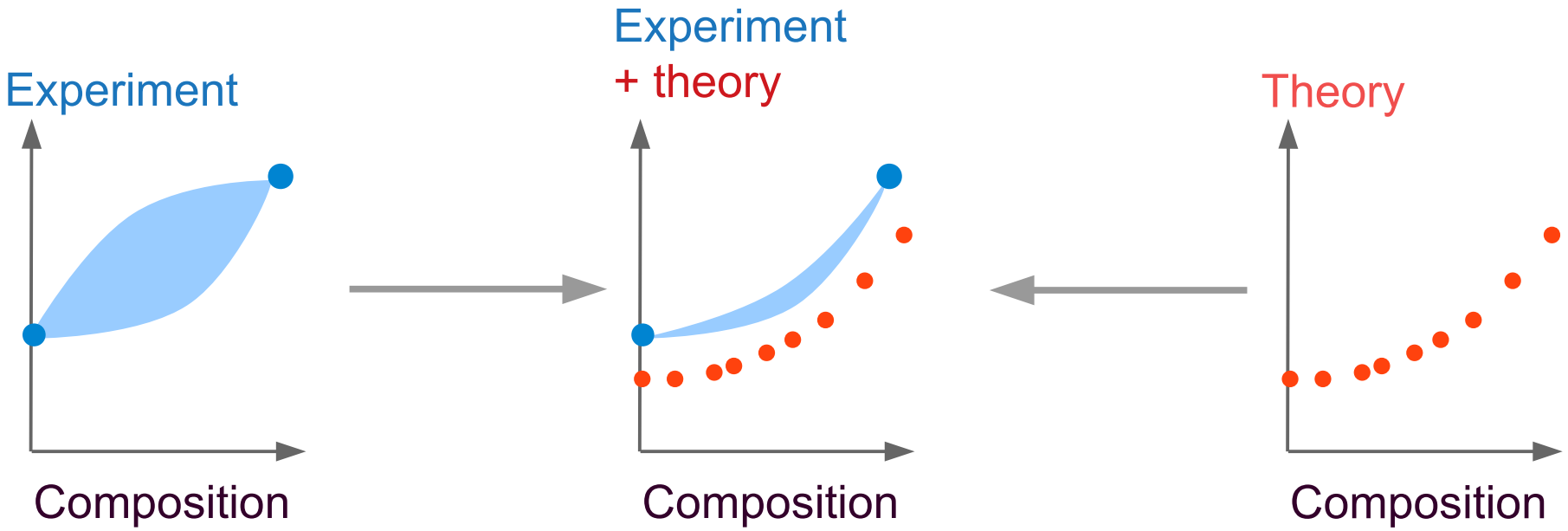


Further information is provided by a simulation

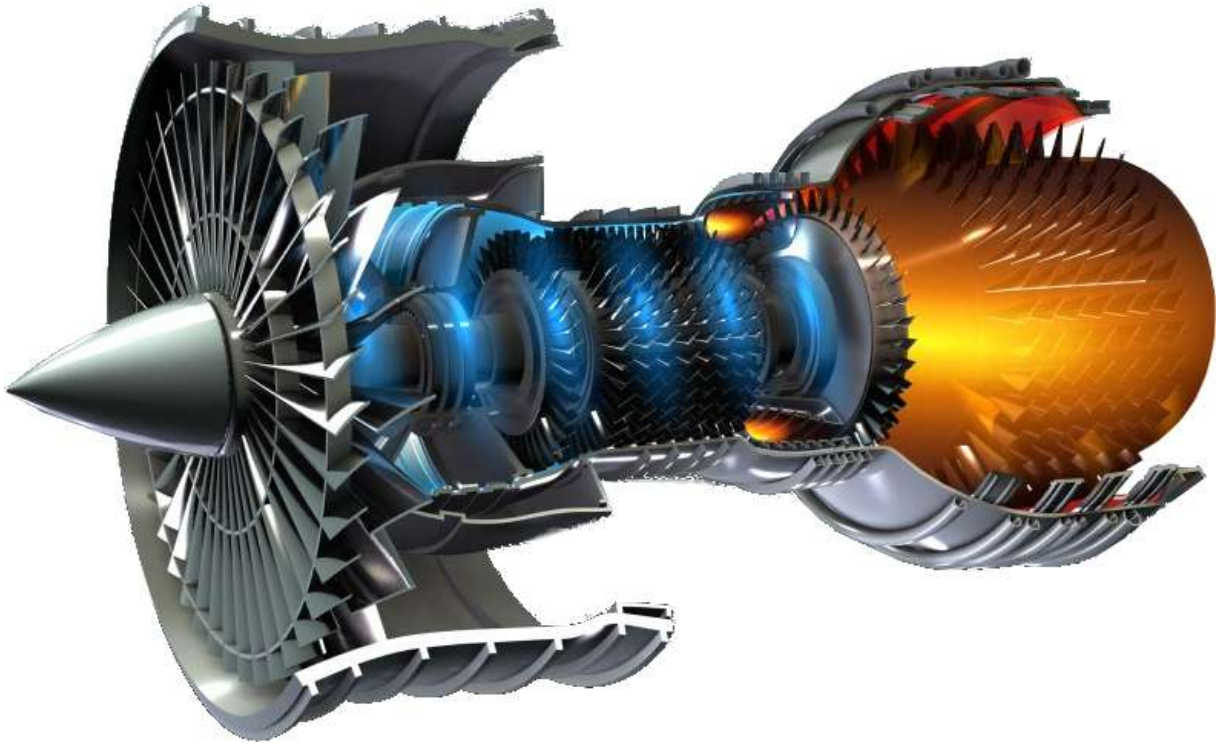




Neural network combines the two sources of data



Schematic of an engine



Target properties

Cost	< 33.7 $\$kg^{-1}$
Density	< 8281 kgm^{-3}
γ’ content	< 50.4 vol%
Phase stability	> 99.0 vol%
Fatigue life	> $10^{3.9}$ cycles
Yield stress	> 752.2 MPa
Ultimate tensile strength	> 960.0 MPa
300hr stress rupture	> 674.5 MPa
Cr activity	> 0.14
γ’ solvus	> 983ºC
Tensile elongation	> 11.6%

Proposed alloy

Cr:15.8

Co: 20.0

Mo: 0.5

W: 0.5

Ta: 4.9

Nb: 1.1

Al: 2.4

Ti: 3.0

Fe: 3.9

Mn: 0.2

Si: 0.2

C: 0.02

B: 0.06

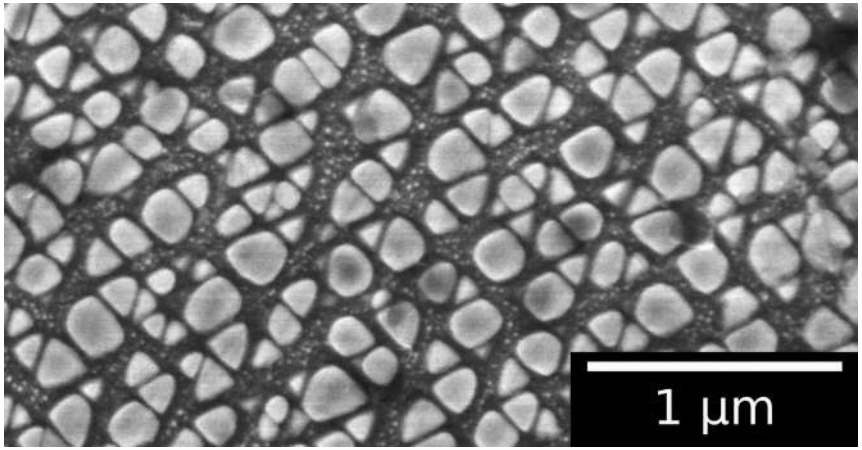
Zr: 0.18

Ni: 47.2

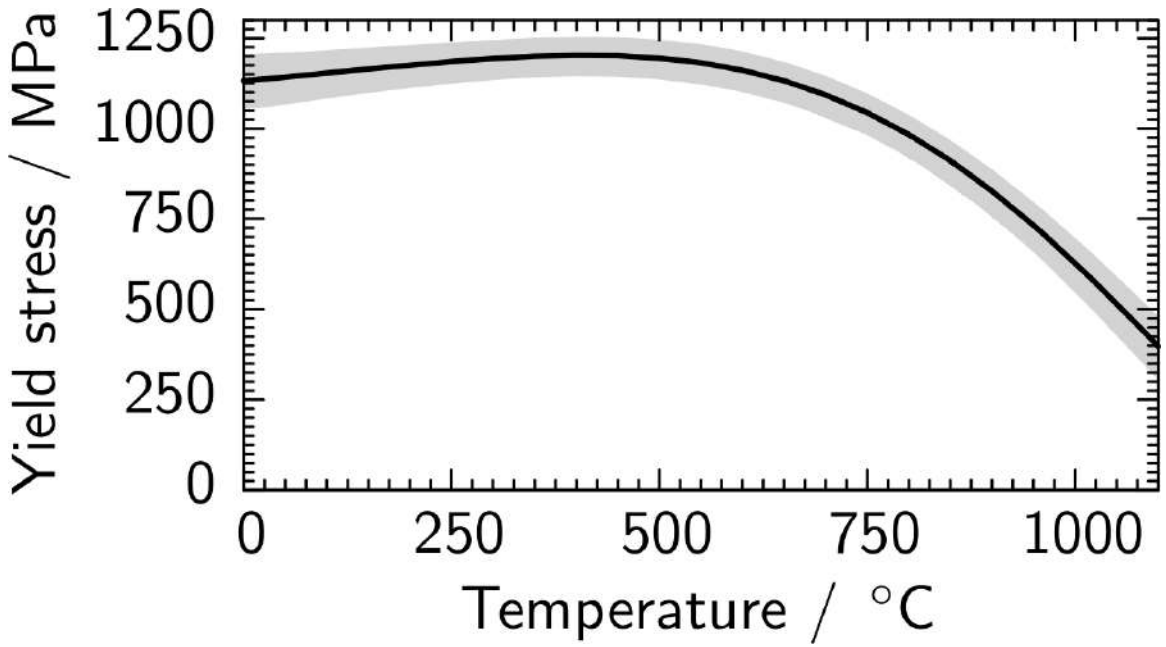
900ºC

30 hours

Microstructure

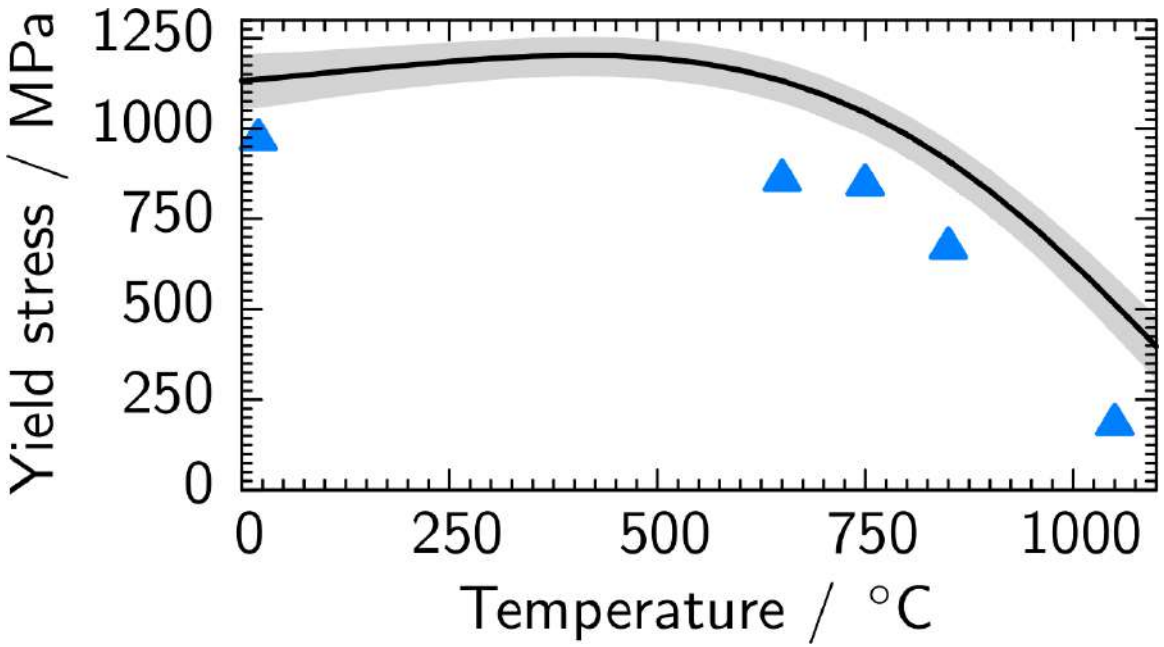


Predict the yield stress



Proposed theory

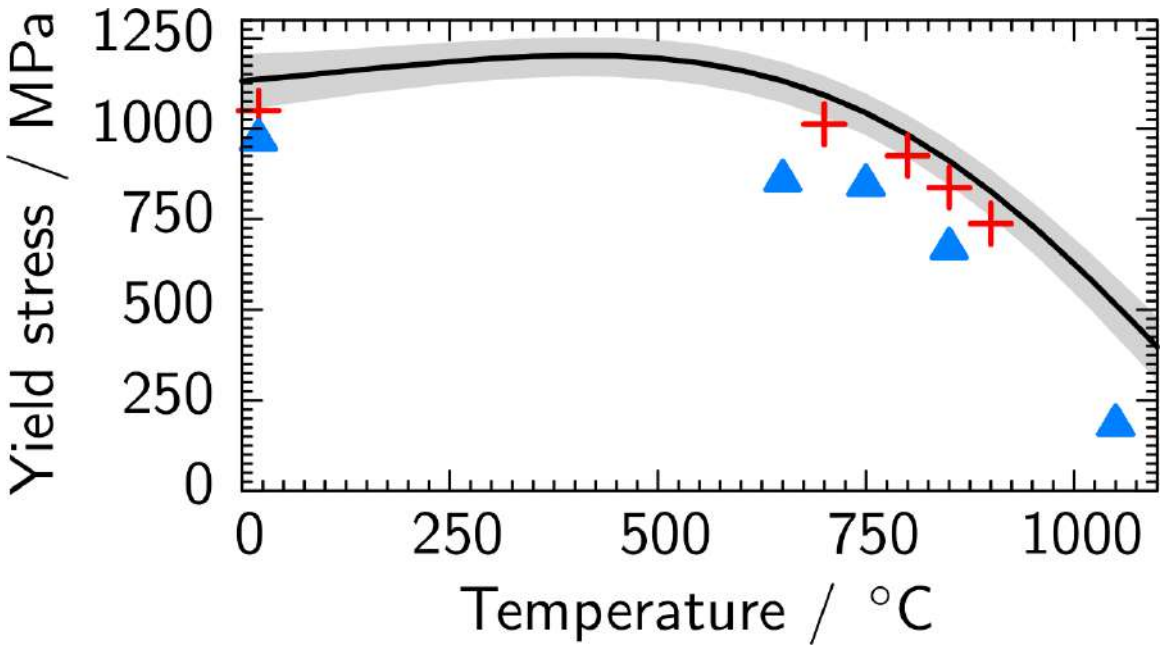
Test the yield stress



Proposed theory

RR1000

Test the yield stress

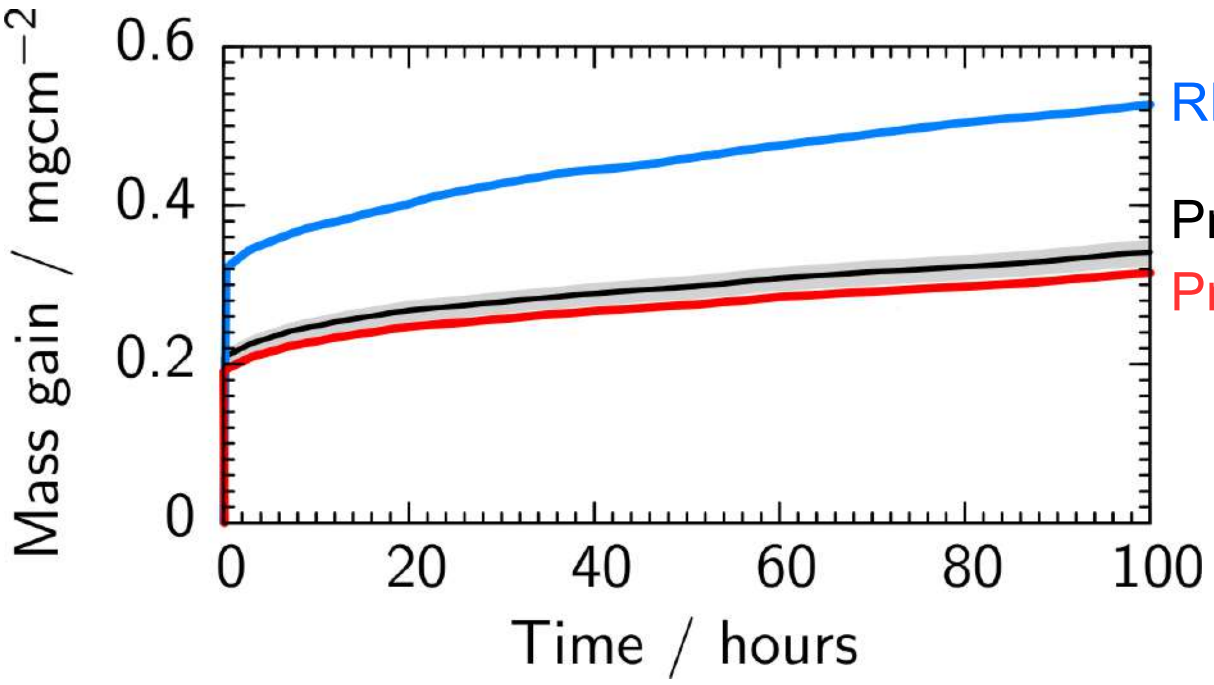


Proposed theory

Proposed experiment

RR1000

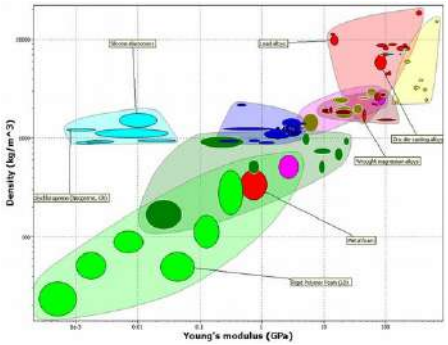
Test the oxidation resistance



More materials designed

3D printed alloy designed from 7 data entries

Identified and corrected errors in materials database



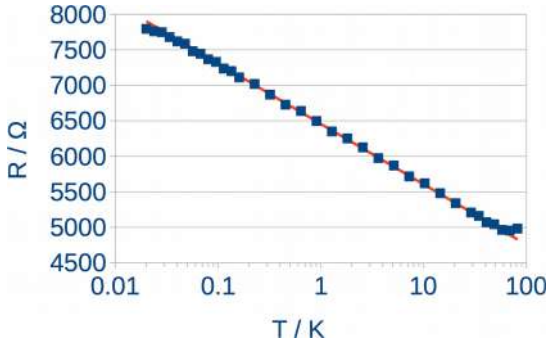
Battery design with DFT and experimental data

Even more materials designed

Designing lubricants with DFT and experimental data

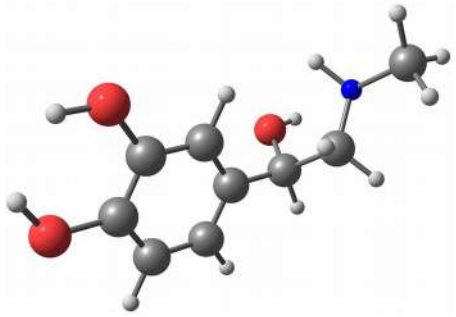
bp

Thermometer with quantum and experimental data



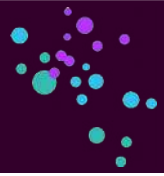
Lake Shore CRYOTRONICS

Drug design



e-therapeutics

Steel demo http://app.intellegens.ai/app/network/#/327



CARBON AND LOW-ALLOY STEELS

This network can be used for carbon steels and low-alloy steels containing only the alloying elements listed below, within the specified ranges. The predicted values represent typical properties for the wrought and annealed condition. Composition should be entered in weight %

Name	Input	
C (carbon)		(0.0 - 0.965)
Cr (chromium)		(0.0 - 1.2)
Mn (manganese)		(0.0 - 1.75)
Mo (molybdenum)		(0.0 - 0.25)
Ni (nickel)		(0.0 - 3.5)
Si (silicon)		(0.0 - 0.25)
Young's modulus		(205.1 - 213.0)
Yield strength (elastic limit)		(134.7 - 469.6)
Tensile strength		(260.5 - 815.6)
Elongation		(12.6 - 43.9)
Fracture toughness		(52.4 - 166.5)
Thermal conductivity		(39.7 - 75.3)
Specific heat capacity		(434.3 - 499.6)
Thermal expansion coefficient		(11.0 - 13.2)

Summary: future prospects

Apply deep learning to high-value fragmented data

Merge experiments and simulations into holistic design tool

Experimentally proven materials and drugs design with 7 companies, founded startup intellegens.ai

Steels demonstrator: http://app.intellegens.ai/app/network/#/327