UNIVERSITY OF CAMBRIDGE

Who needs atoms to design materials?

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Theory of Condensed Matter Group, Department of Physics

A deep neural network algorithm that

Merge simulations, physical laws, and experimental data

Reduces need for expensive experimental development

Accelerate materials discovery

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

Neural networks: first train

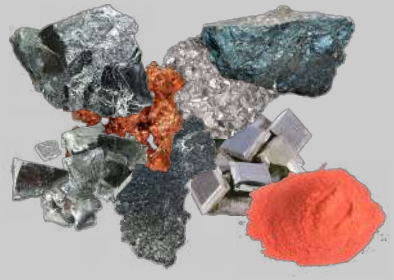
Neural networks: then predict

Unique neural network: train on fragmented data

Unique neural network: predict on fragmented data

Neural networks for materials design

Composition



Artificial intelligence

Properties

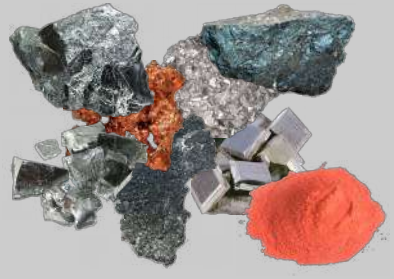
UTS

Hardness

Cost

Neural networks for materials design

Composition



Properties

UTS

Hardness

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Simulations

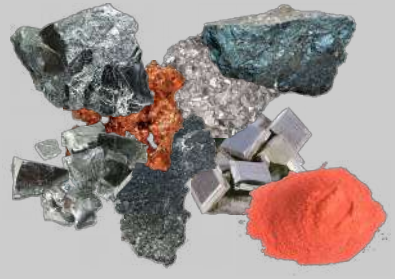
Density Functional

Molecular dynamics

Finite element

Artificial intelligence

Composition



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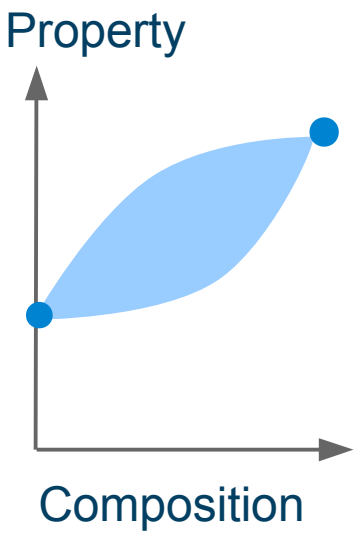
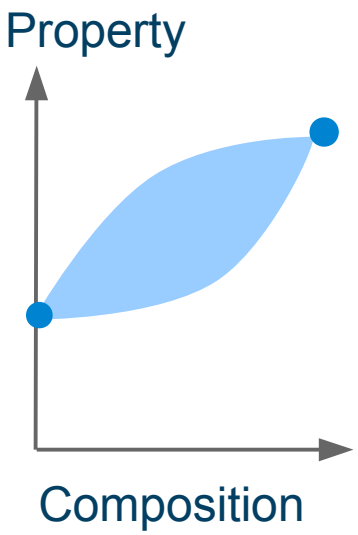
Combine databases with neural networks

Experiment

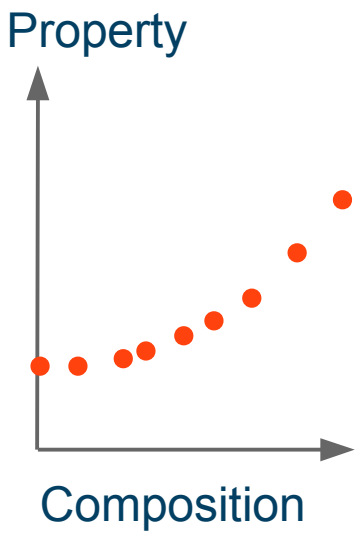


Combine databases with neural networks

Experiment



Simulation

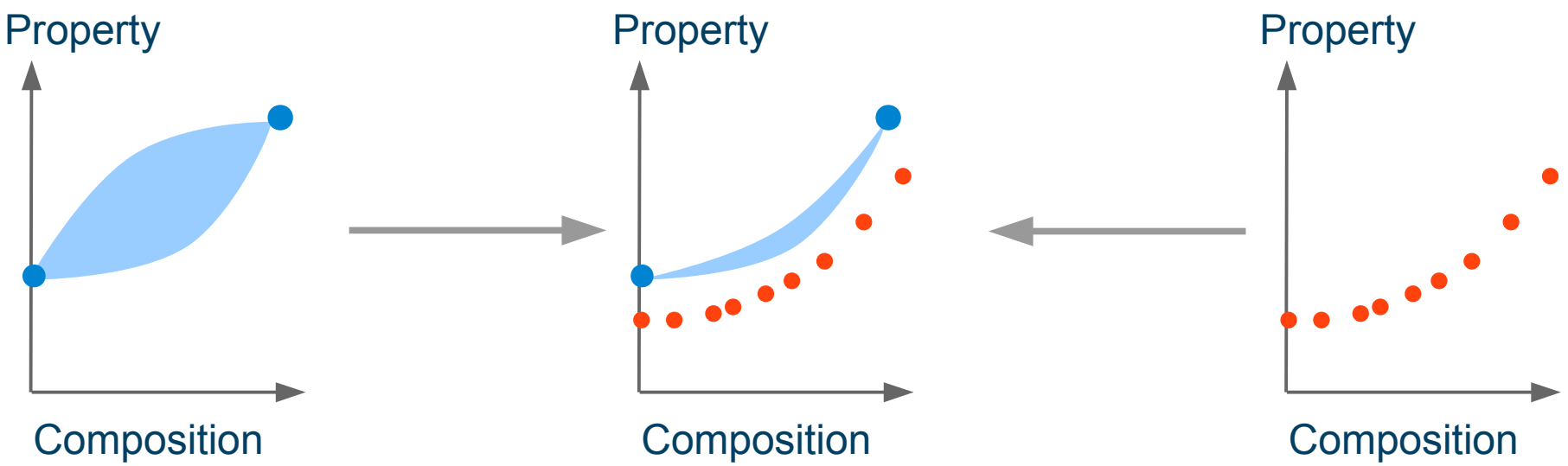


Combine databases with neural networks

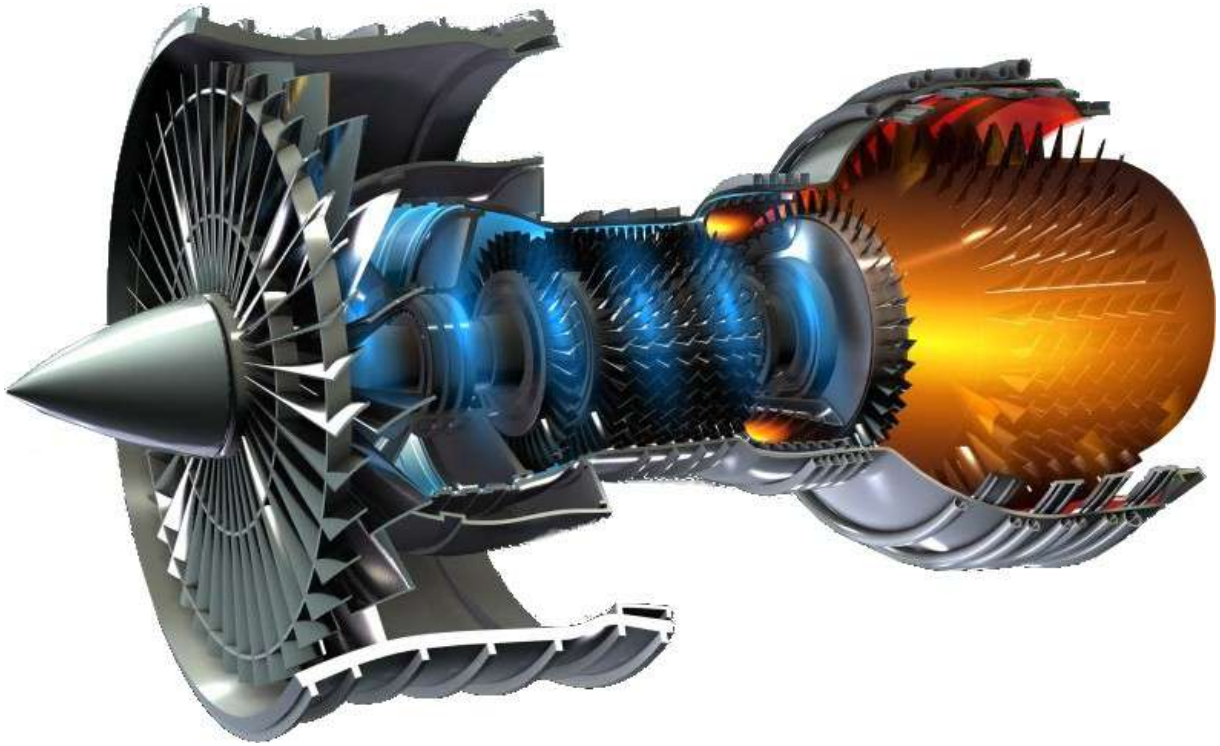
Experiment

Combined

Simulation



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

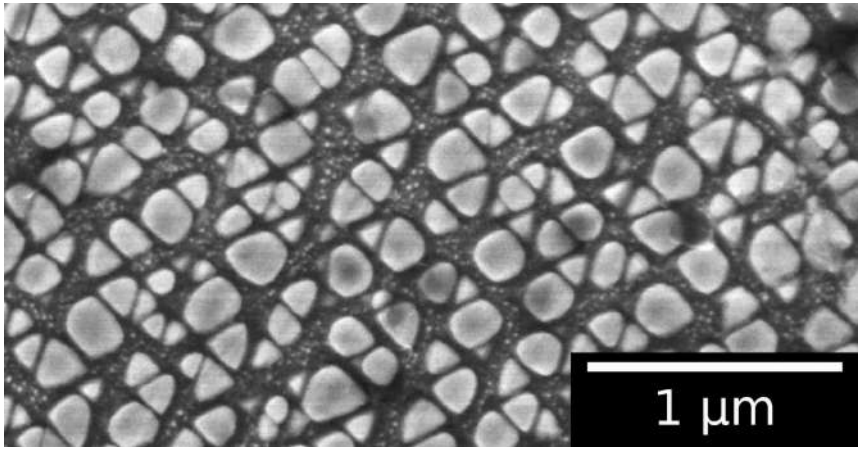
Zr: 0.18

Ni: 47.2

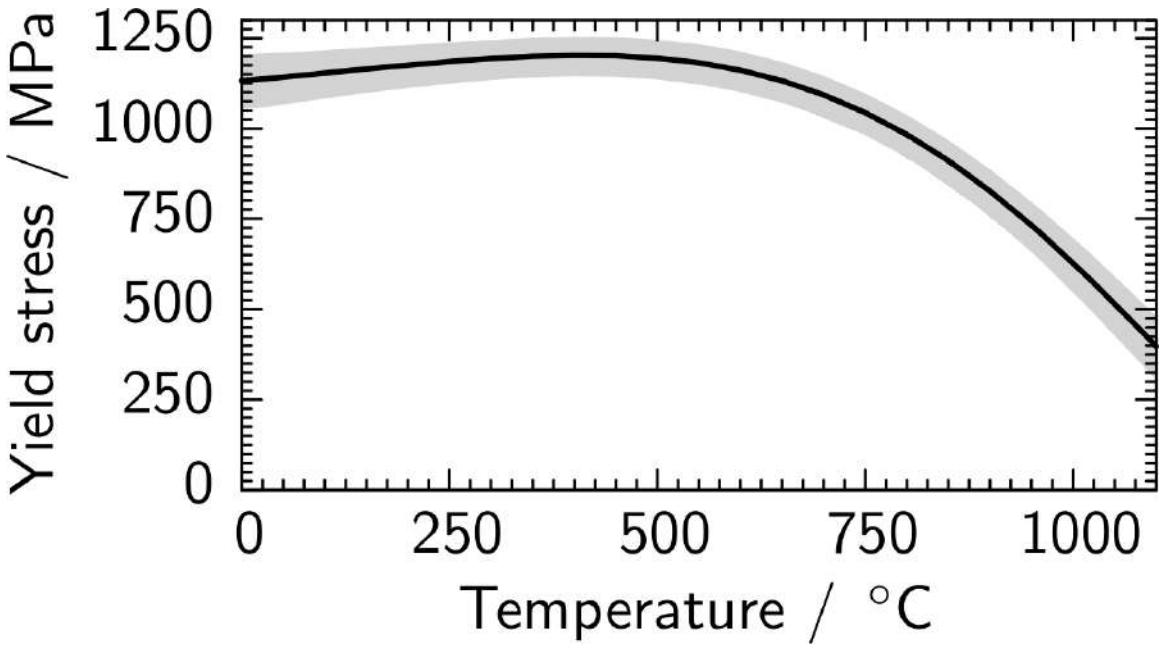
900ºC

30 hours

Microstructure

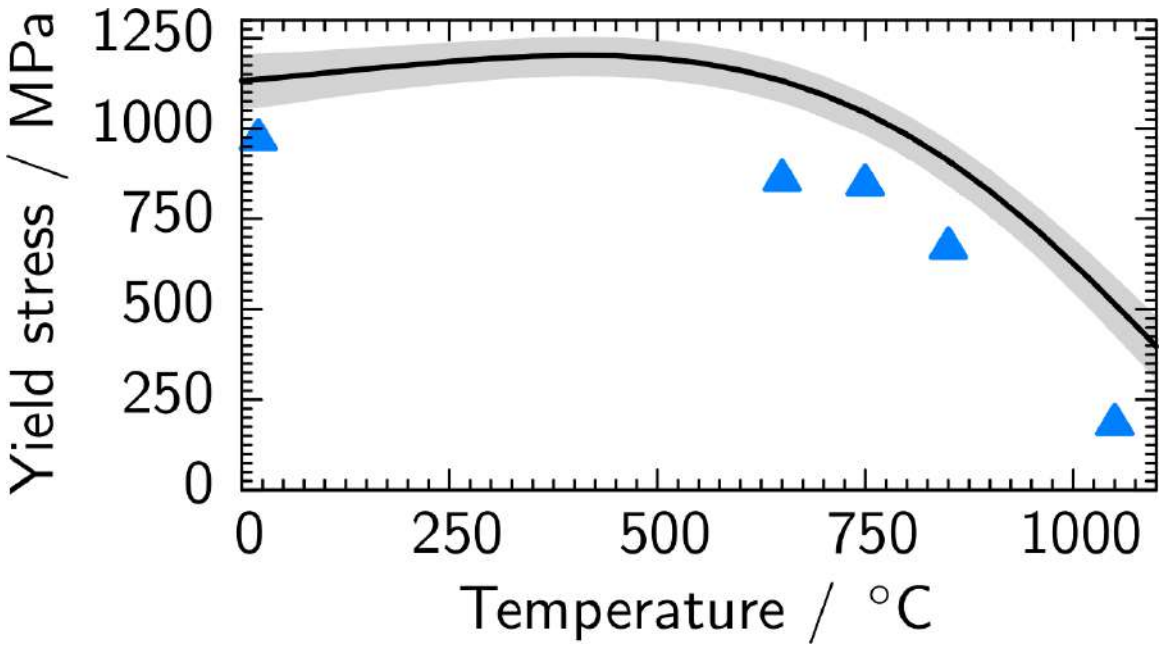


Testing the yield stress



Proposed theory

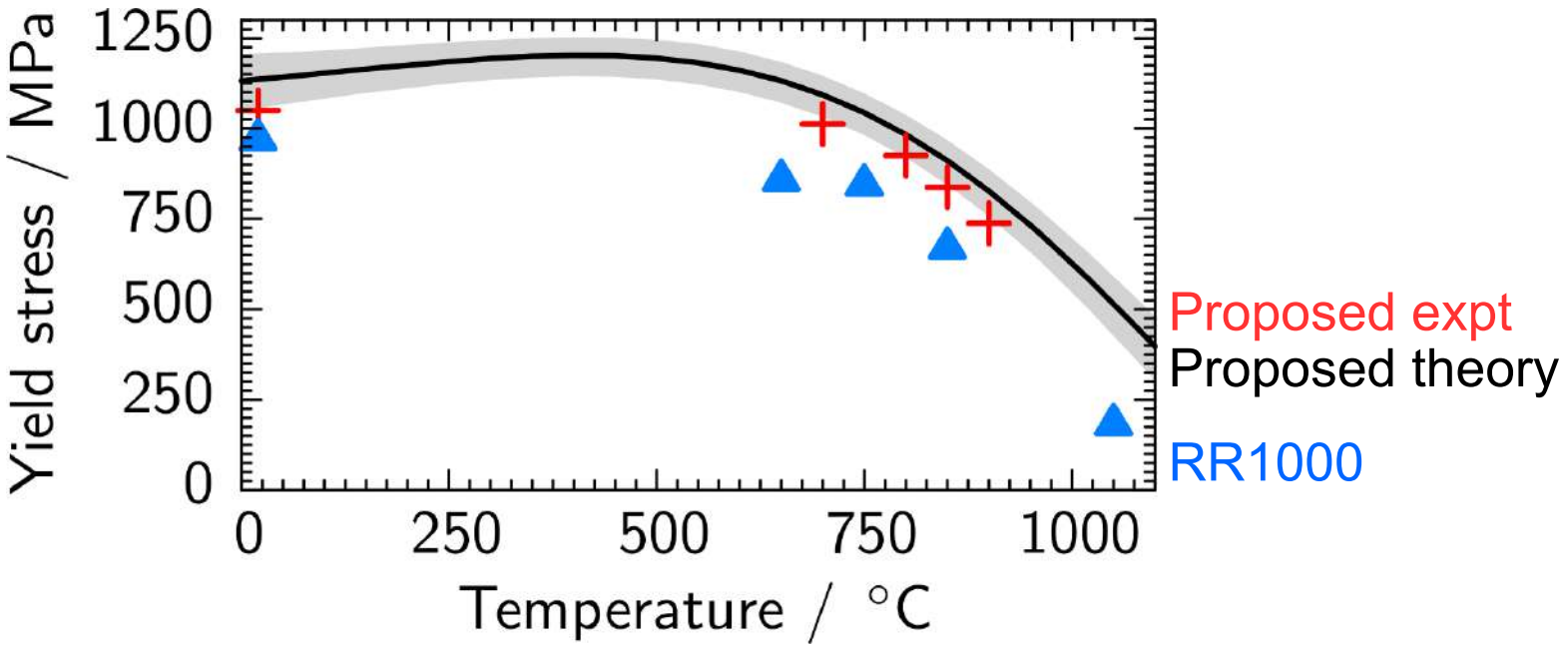
Testing the yield stress



Proposed theory

RR1000

Testing the yield stress



Drug discovery

10,000 proteins with 2,000,000 compounds

Original dataset 0.05% complete

Filled 32% of the entries

Drug discovery with additional data

Include drug structural information to fill to 46%

Saved >$1billion in experimental costs

Summary: progress

Apply deep learning to high-value fragmented data

Experimentally proven materials design with 7 companies, founded startup intellegens

Summary: opportunities

Apply deep learning to high-value fragmented data

Experimentally proven materials design with 7 companies, founded startup intellegens

Merge experiments and simulations into holistic design tool

Summary: challenges

Apply deep learning to high-value fragmented data

Experimentally proven materials design with 7 companies, founded startup intellegens

Merge experiments and simulations into holistic design tool

Establish all possible sources of information