

Materials design with artificial intelligence

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A deep neural network algorithm that

Reduces product development costs

Accelerates product to market

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

Neural networks: first train



Neural networks: then predict



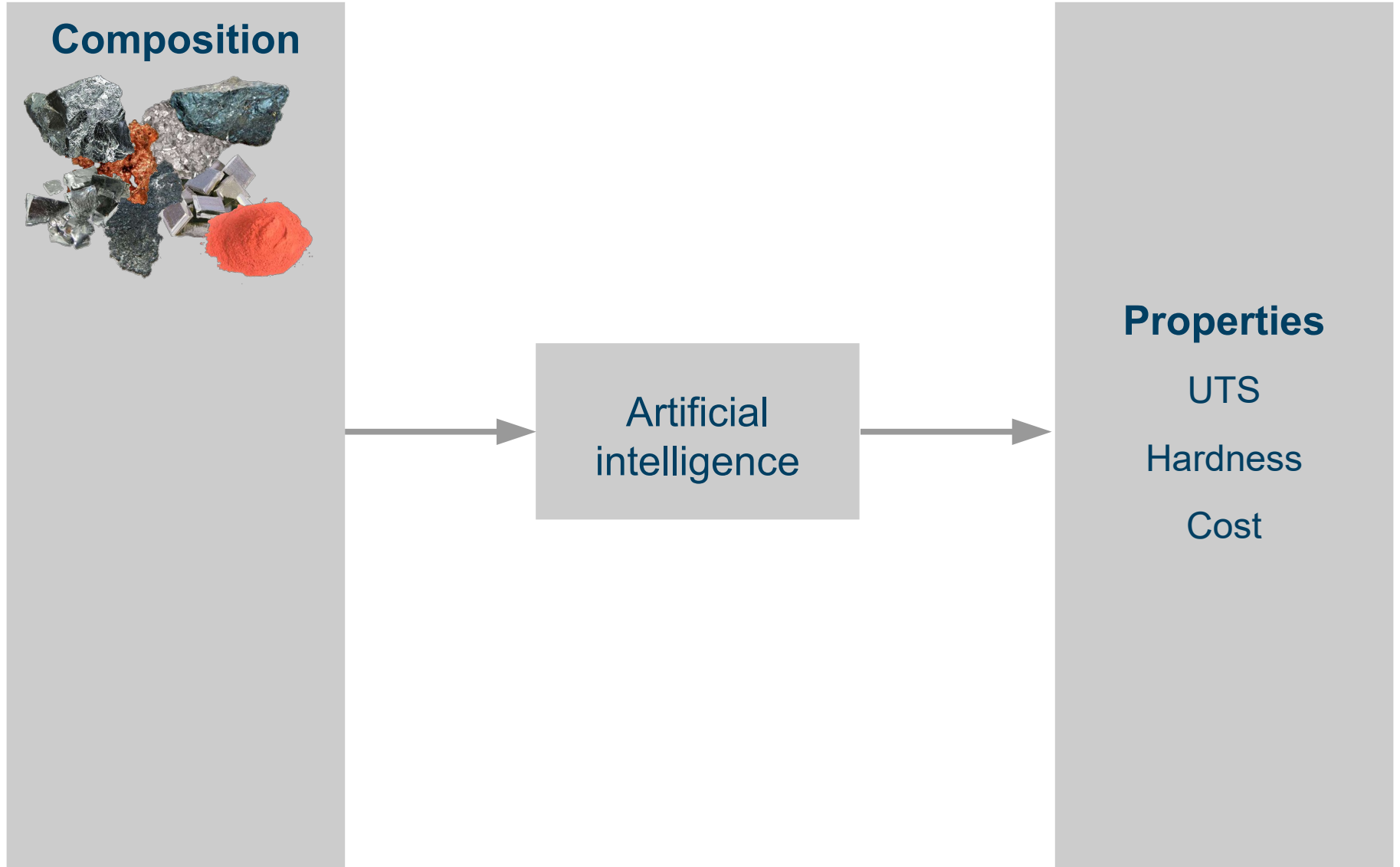
Unique neural network: train on fragmented data



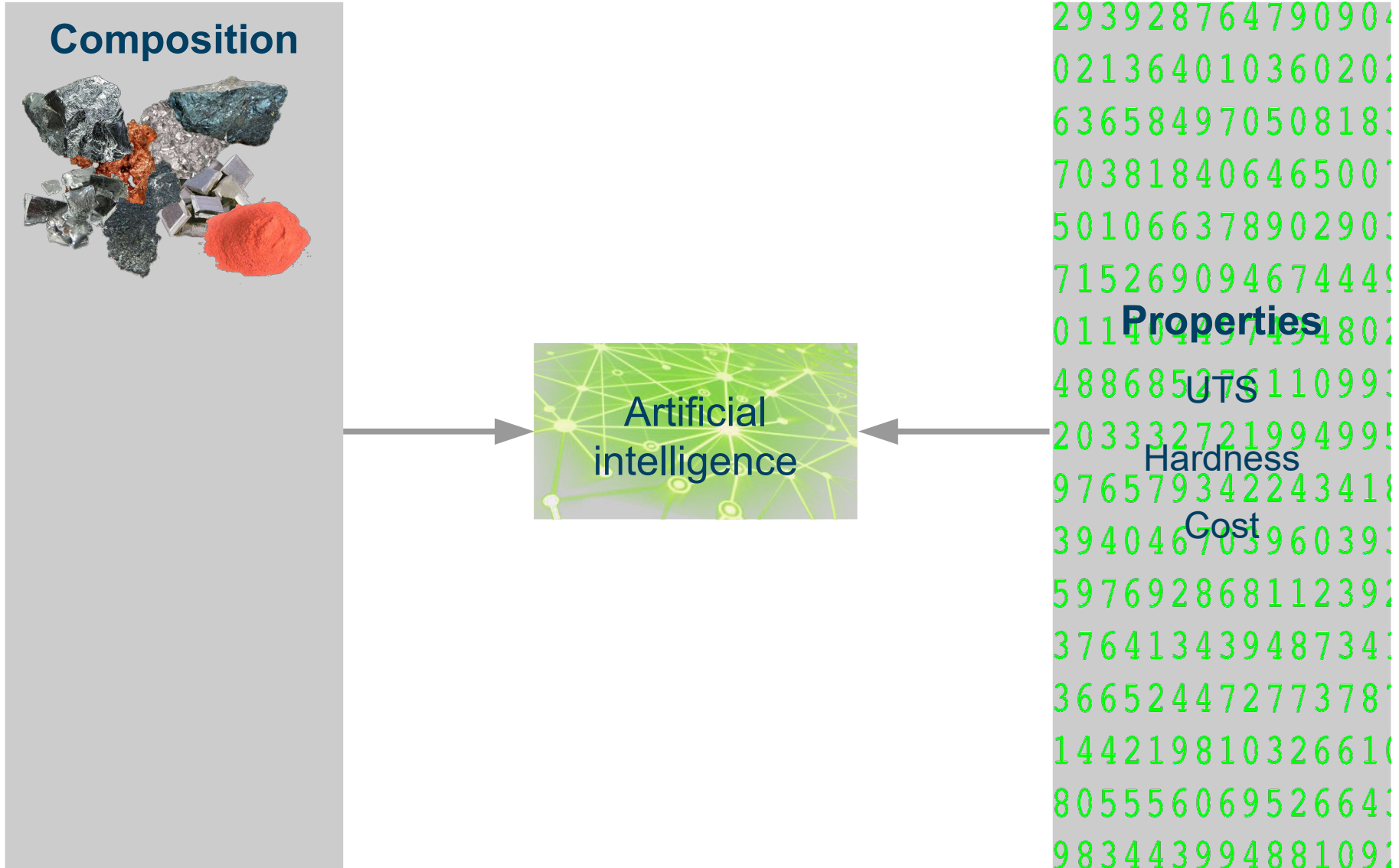
Unique neural network: predict on fragmented data



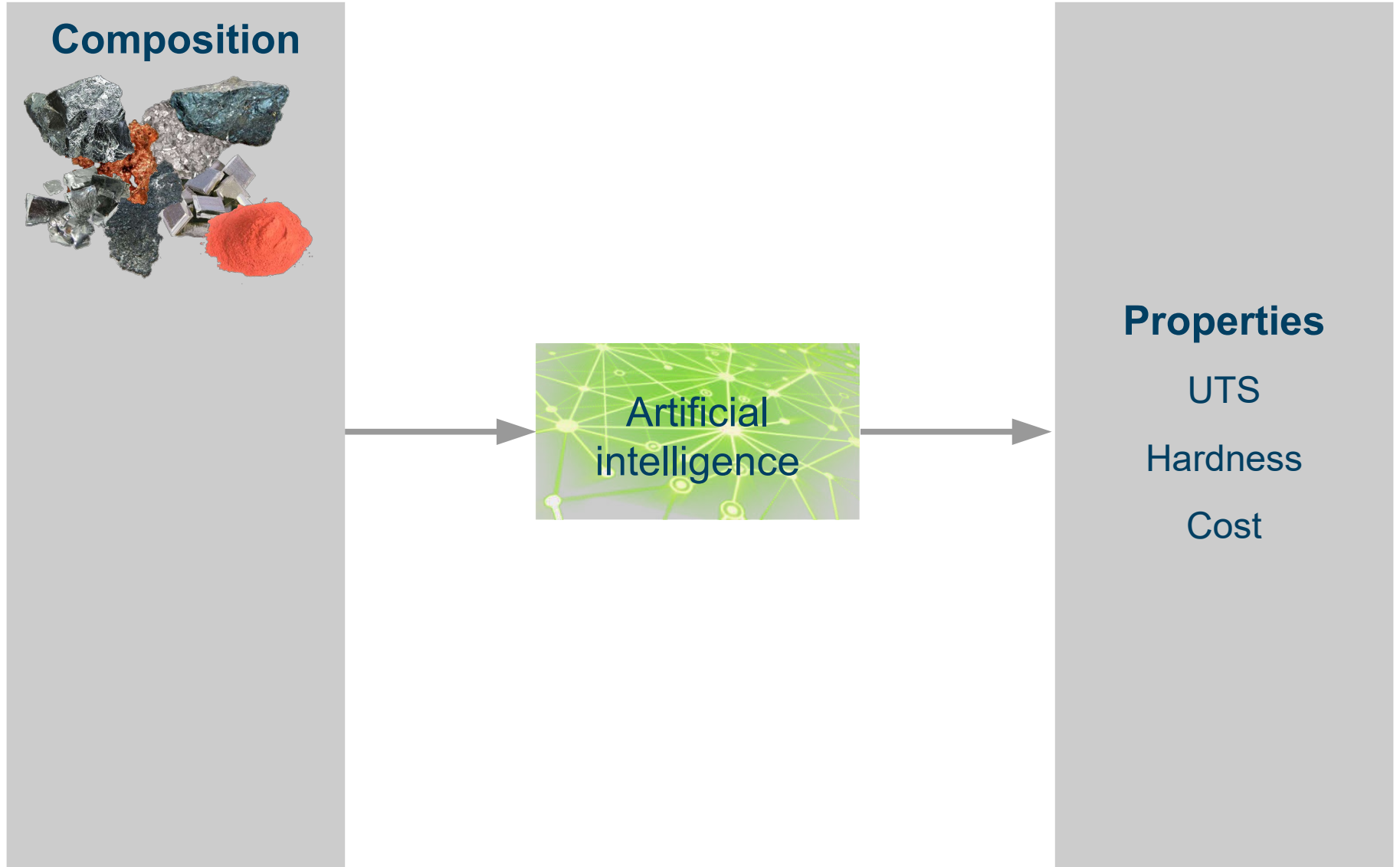
Neural networks for materials design



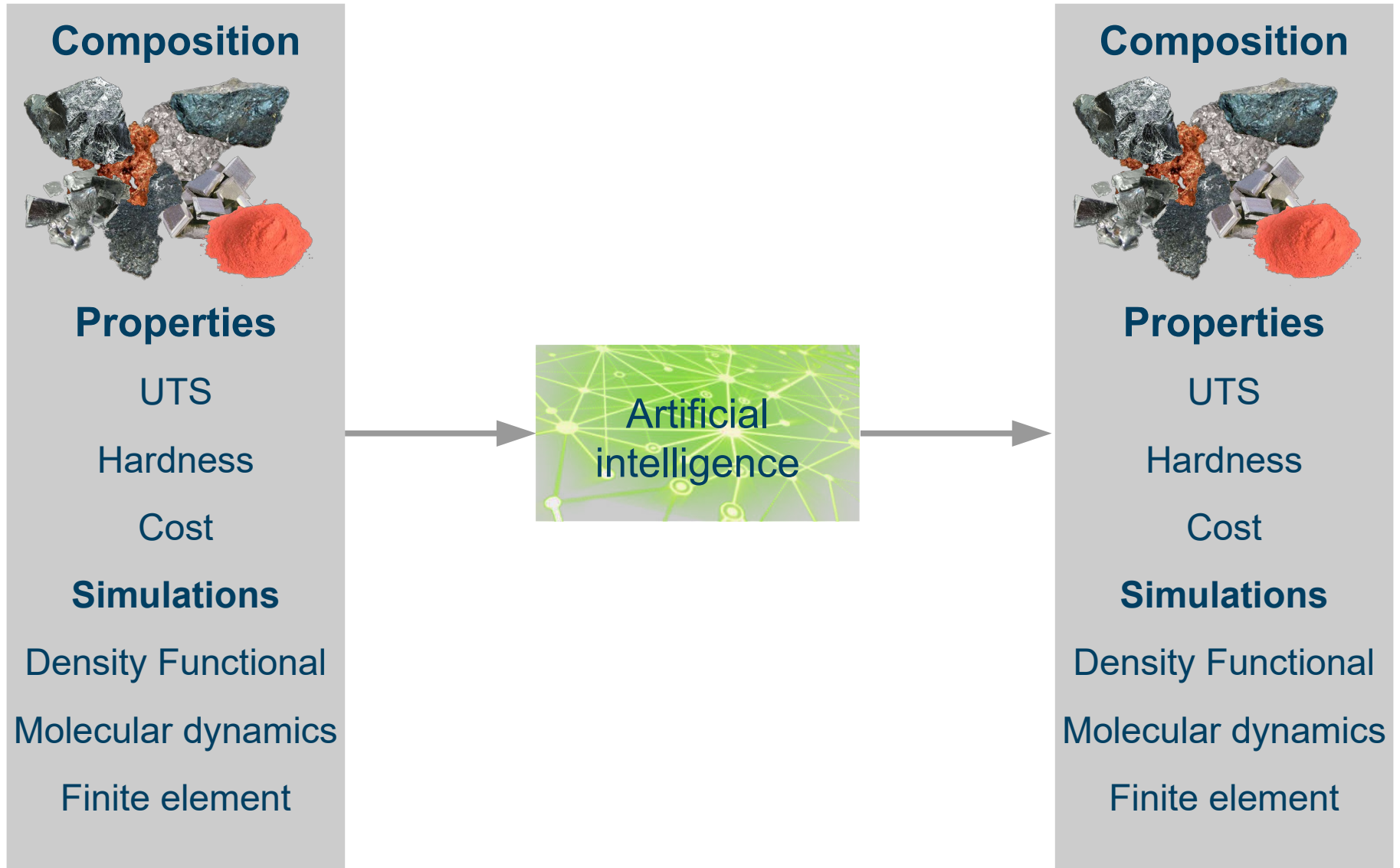
Neural networks for materials design



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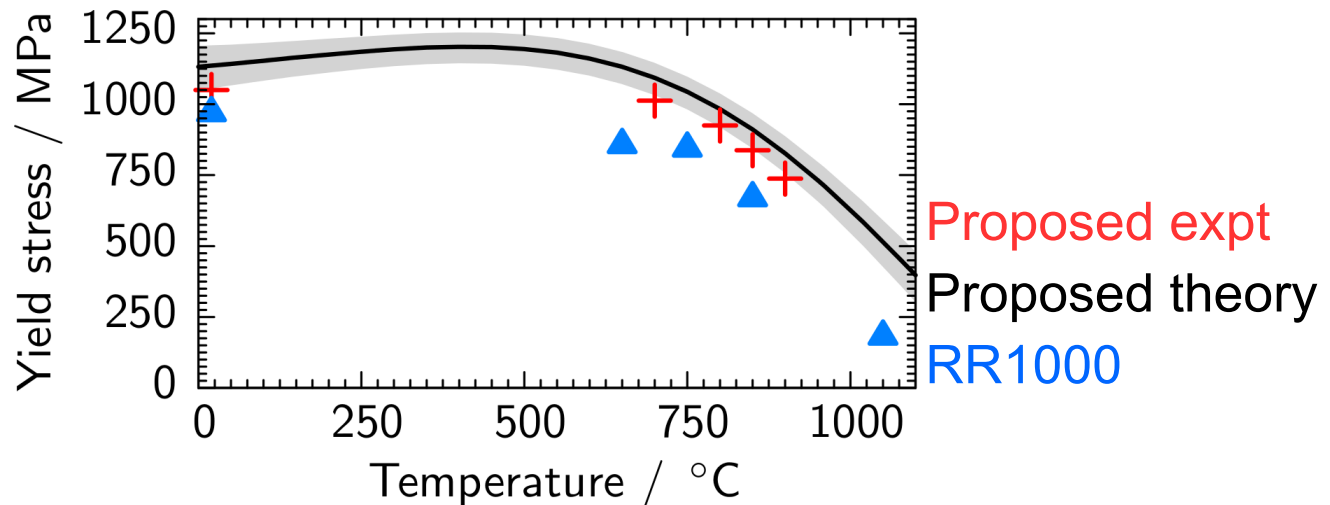


Case study: alloy design with Rolls Royce

Experimental and simulation data for 10,000 alloys

95% fragmented

Design for alloys, experimentally verified and patented



Case study: drug discovery with e-therapeutics

Data for protein activity with compound

Increased drug data available 400-times, saving \$1billion in experimental costs



Materials design

Battery design
with DFT and
experimental data

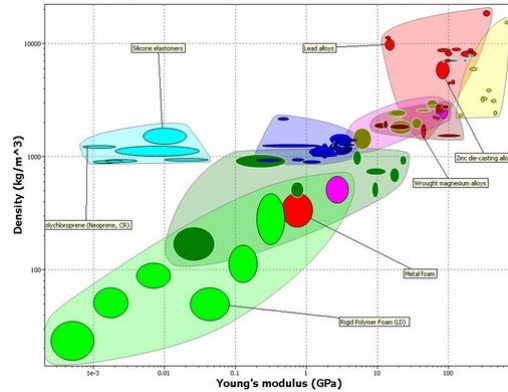


Designing lubricants
with DFT and
experimental data



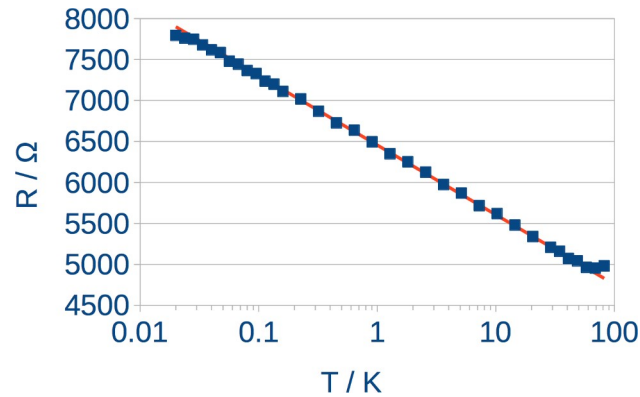
Materials design

Materials databases
Corrected 792 errors



GRANTA
MATERIAL INSPIRATION

Low temperature
thermometer



Lake Shore
CRYOTRONICS

Summary

Apply deep learning to high-value **fragmented** data

Cut costs by reducing need for expensive experiments

Discovery and **verification** in materials and drug discovery

Merge experiments and simulations into **holistic** design tool

Worked with 7 companies, founded startup **intellegens**