UNIVERSITY OF CAMBRIDGE

Materials discovery with artificial intelligence
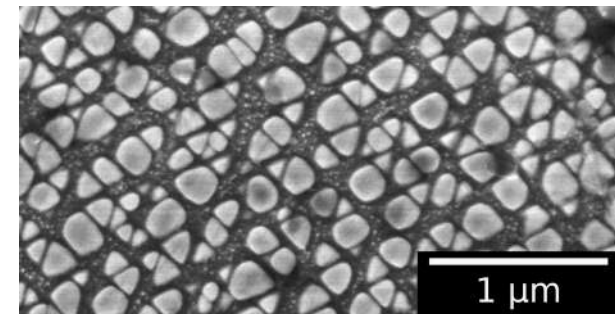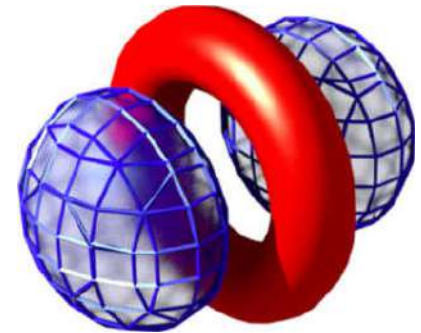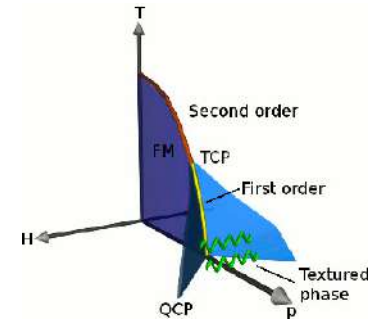
Gareth Conduit
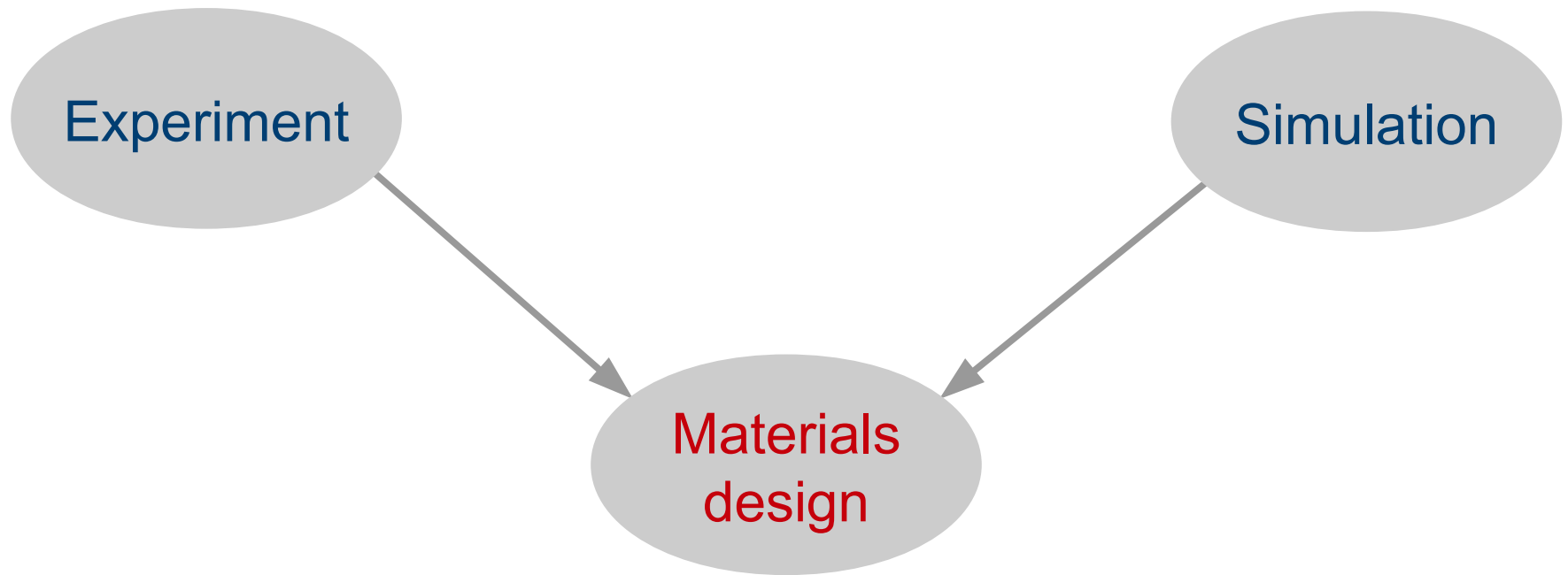
TCM Group, Department of Physics

Cambridge
PhD: Ferromagnets

Weizmann Institute
Royal Commission for the
Exhibition of 1851

Cambridge
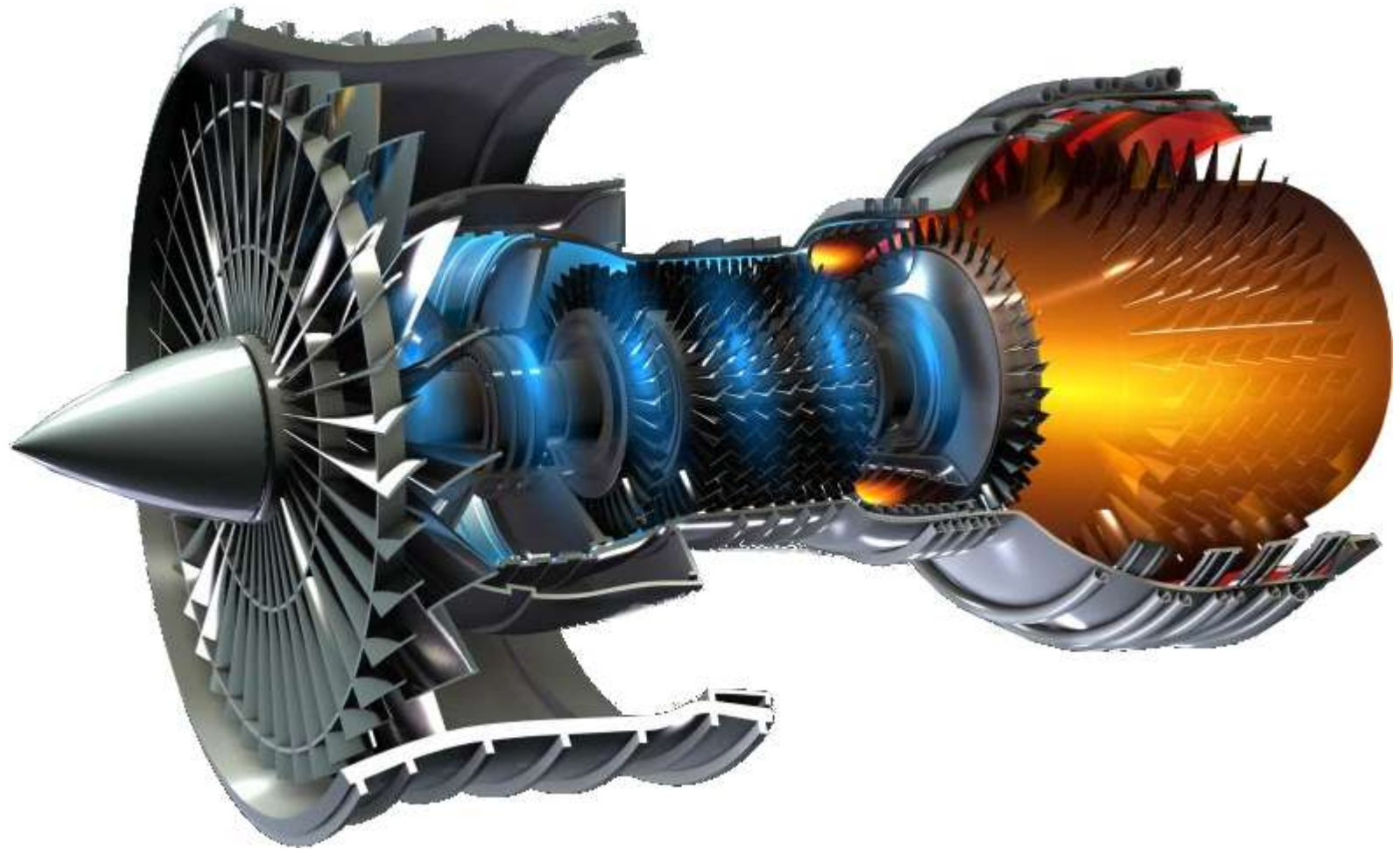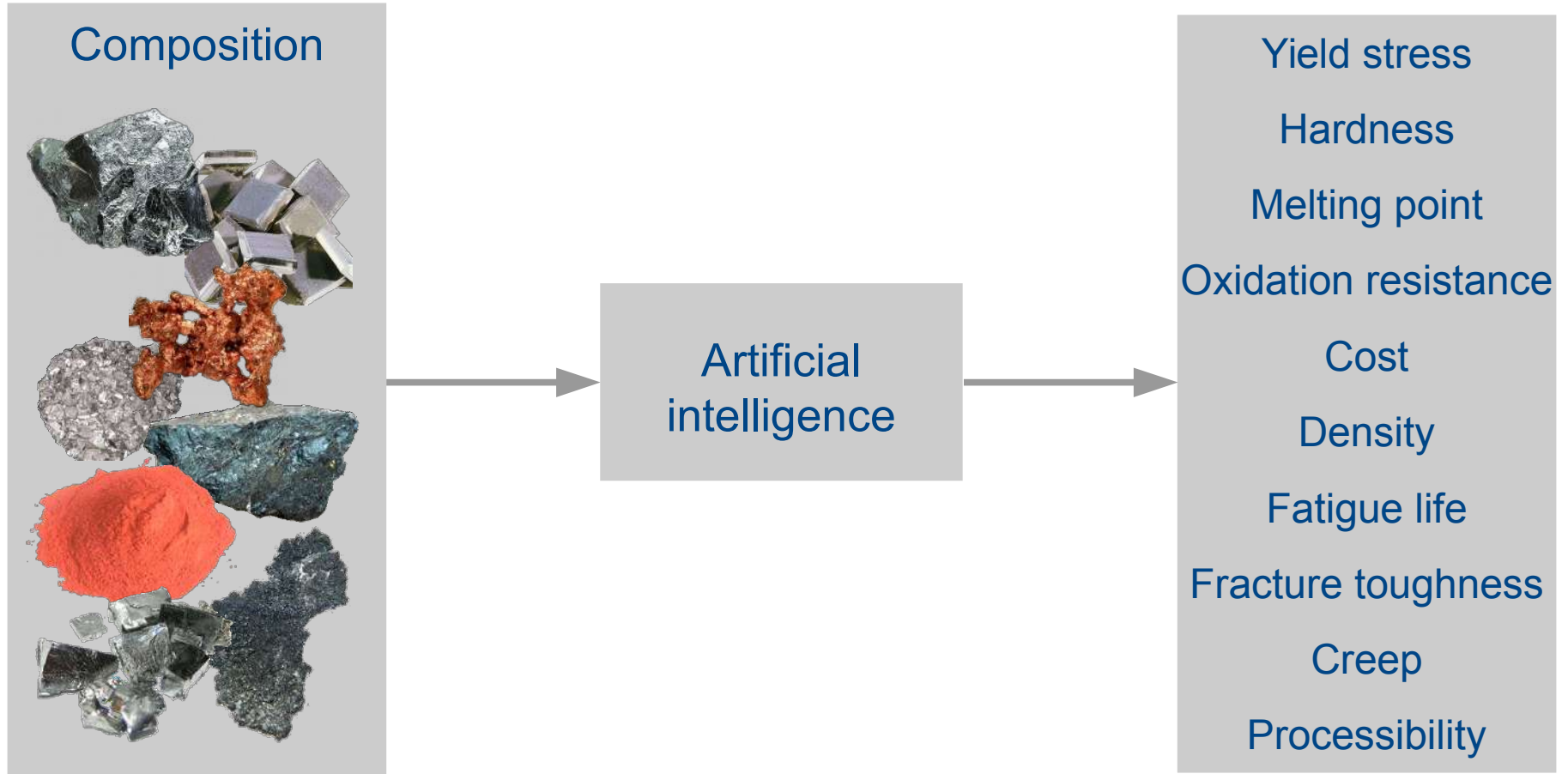Royal Society University
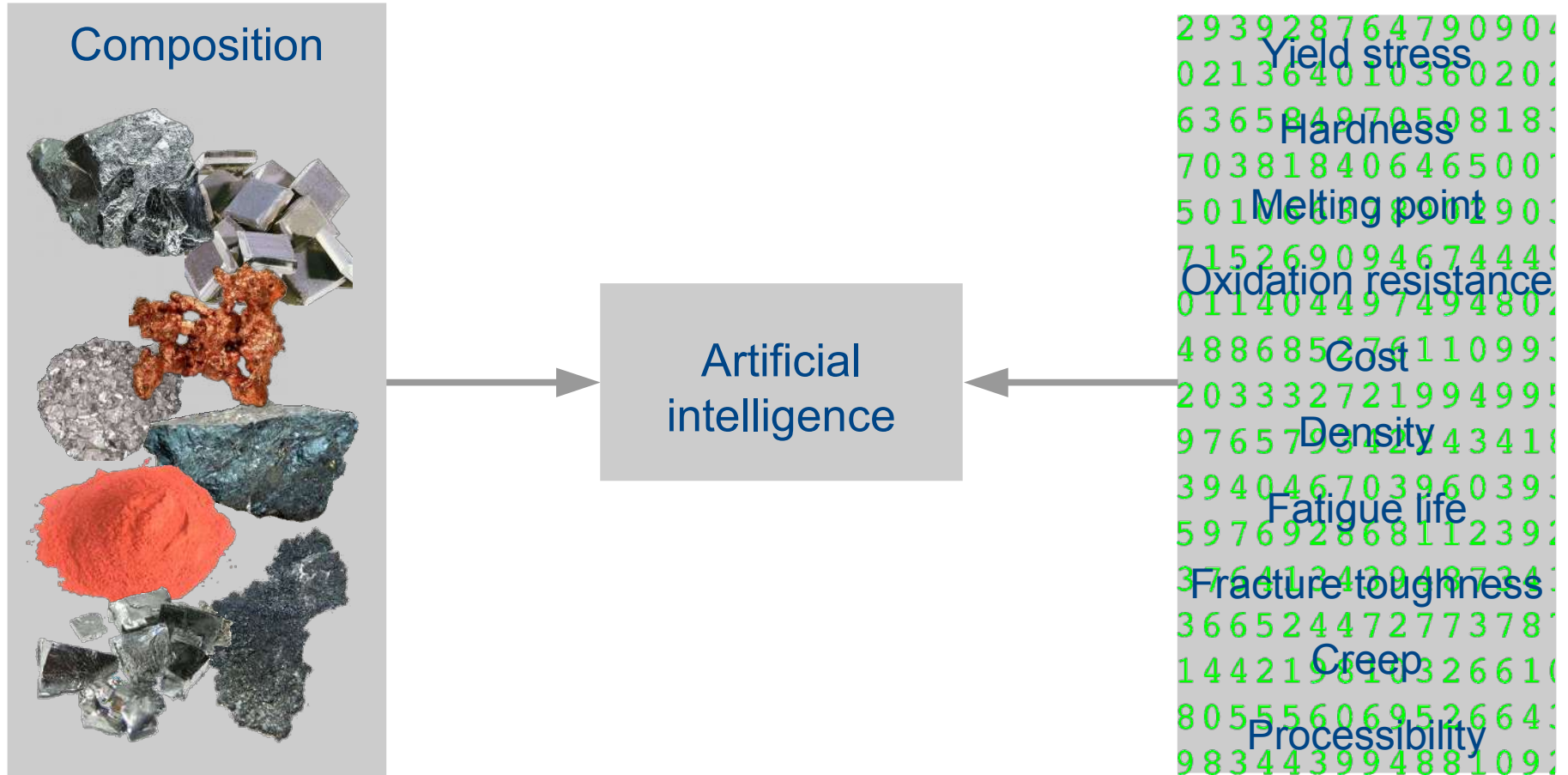Research Fellowship

Approaches to materials design

Experiment

Simulation

Materials design

Schematic of a jet engine

Artificial intelligence

Composition → Artificial intelligence → Yield stress, Hardness, Melting point, Oxidation resistance, Cost, Density, Fatigue life, Fracture toughness, Creep, Processibility

Artificial intelligence

Composition

Artificial intelligence

Yield stress

Hardness

Melting point

Oxidation resistance

Cost

Density

Fatigue life

Fracture toughness

Creep

Processibility

Artificial intelligence

Testing the yield stress

Proposed theory

Testing the yield stress

Proposed theory

RR1000

Proposed expt
Proposed theory
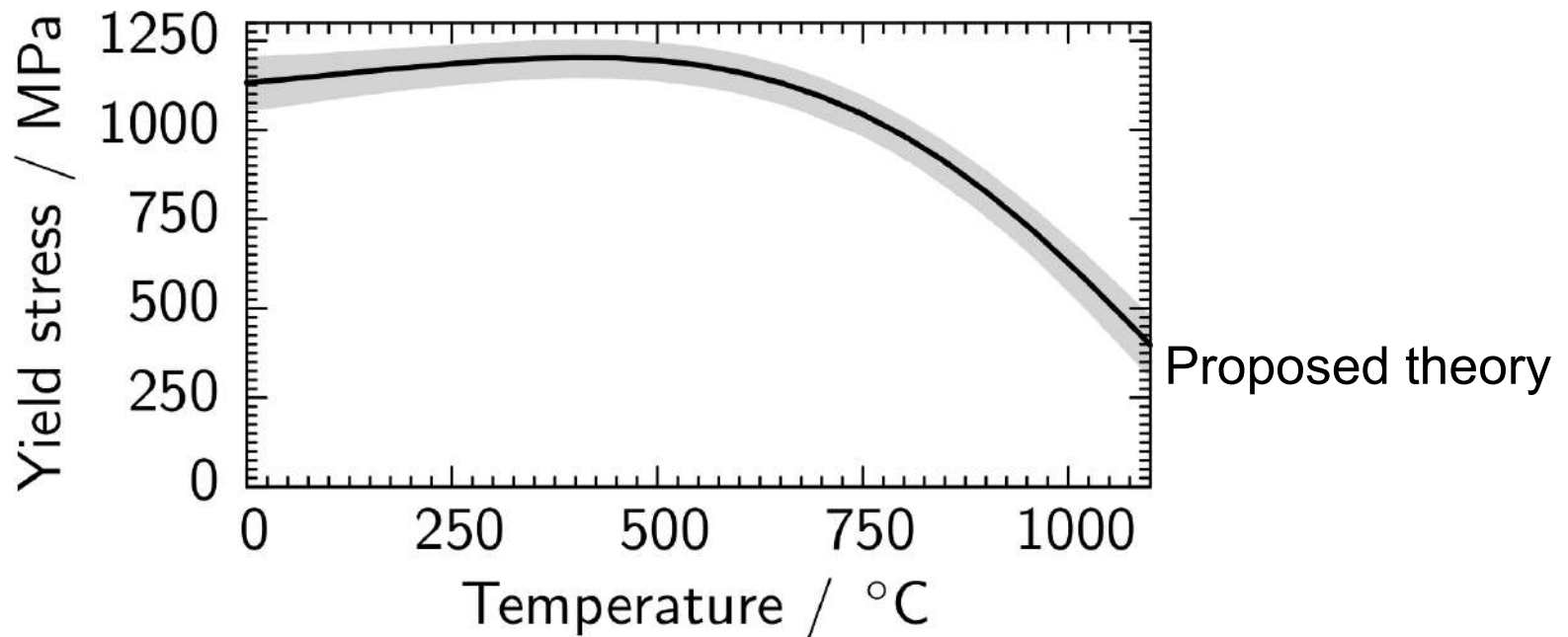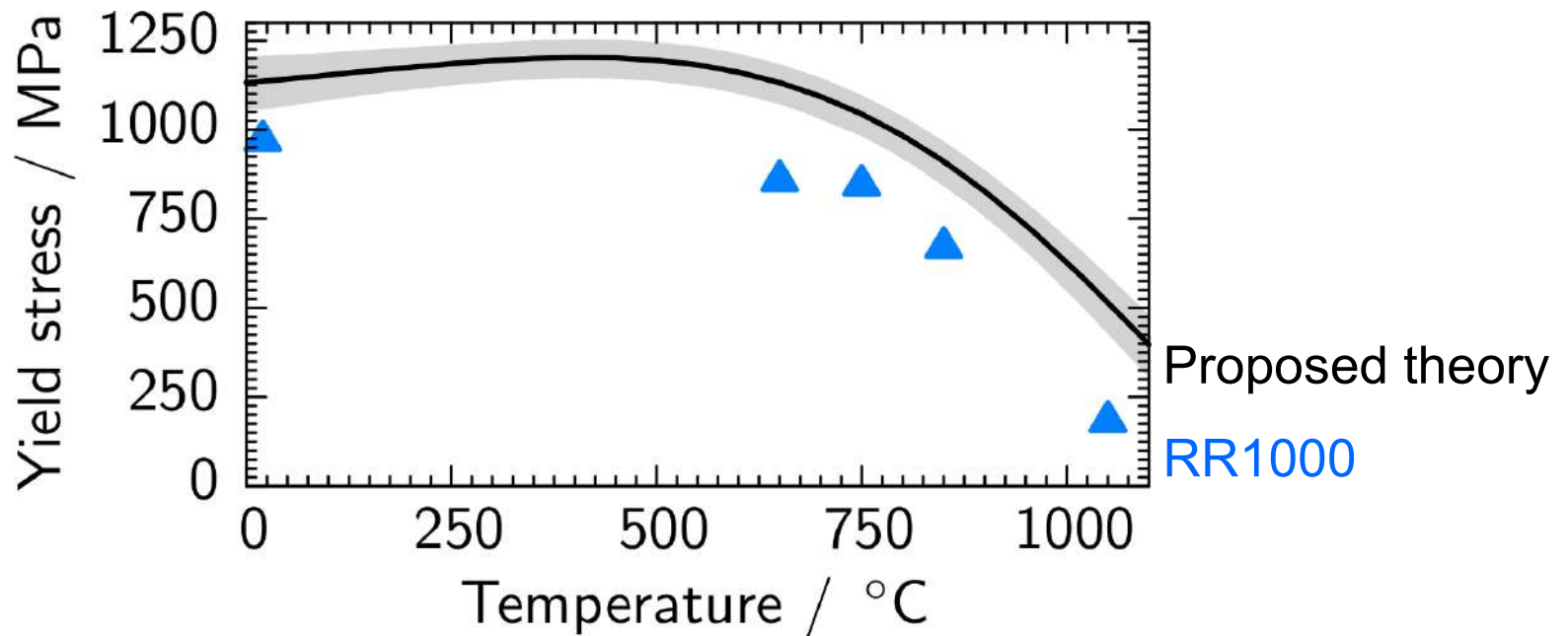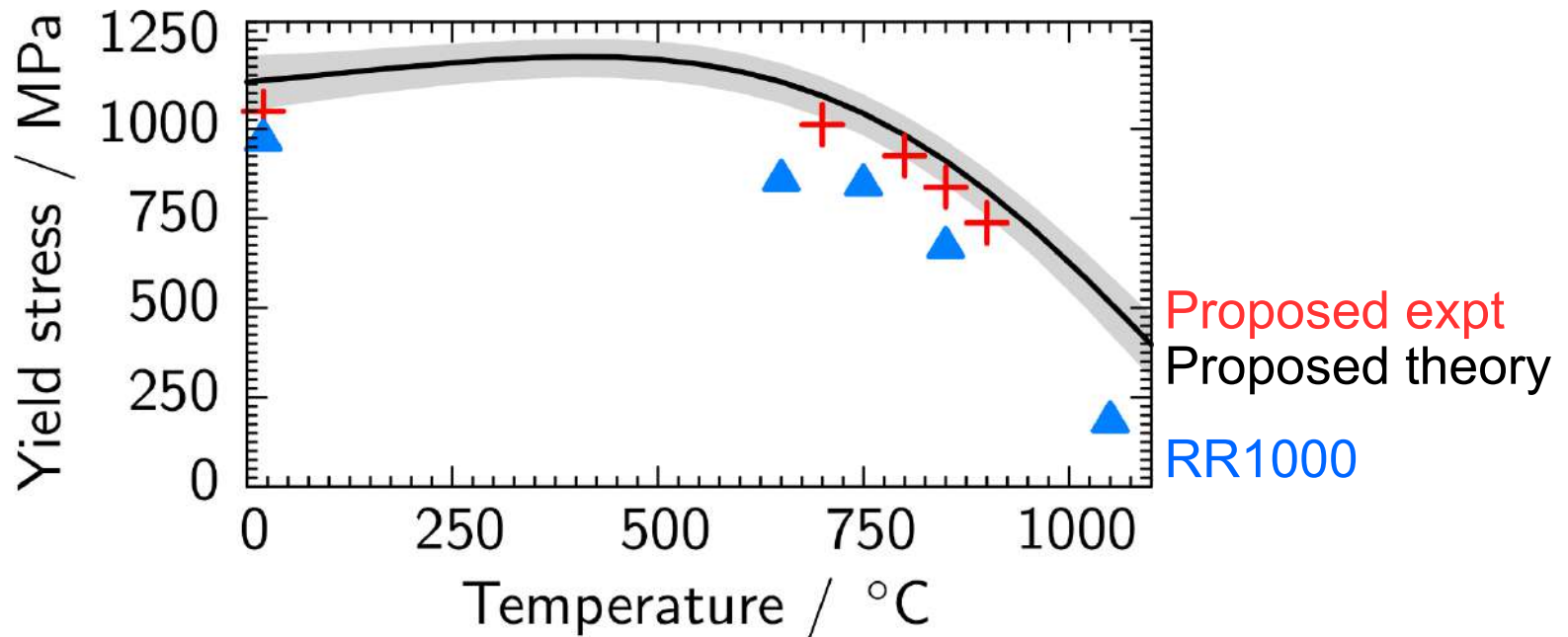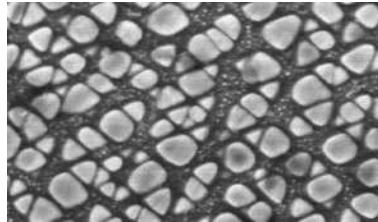
RR1000

Alloys discovered

Cr-Cr$_2$Ta alloys
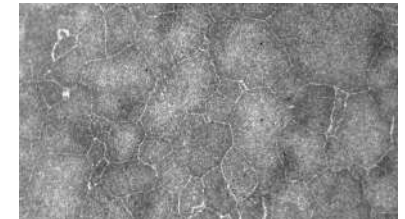Intermetallics, 48, 62
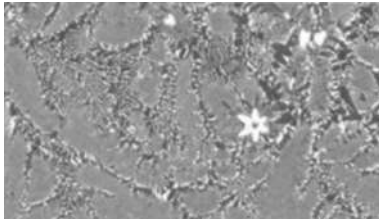
Combustor alloy
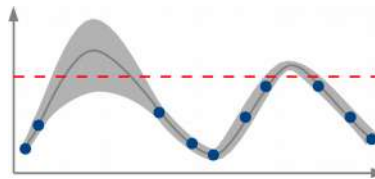GB1408536

RR1000 grain growth
Acta Materialia, 61, 3378
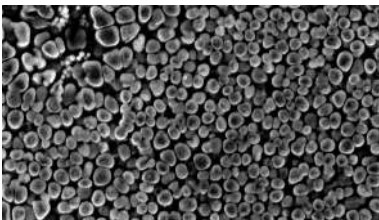

Discovery algorithm
EP14153898
US 2014/177578
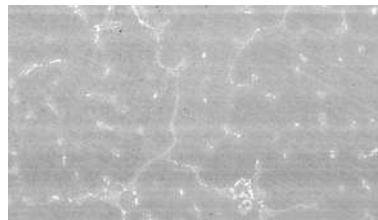

Ni disc alloy
EP14157622
US 2013/0052077 A2

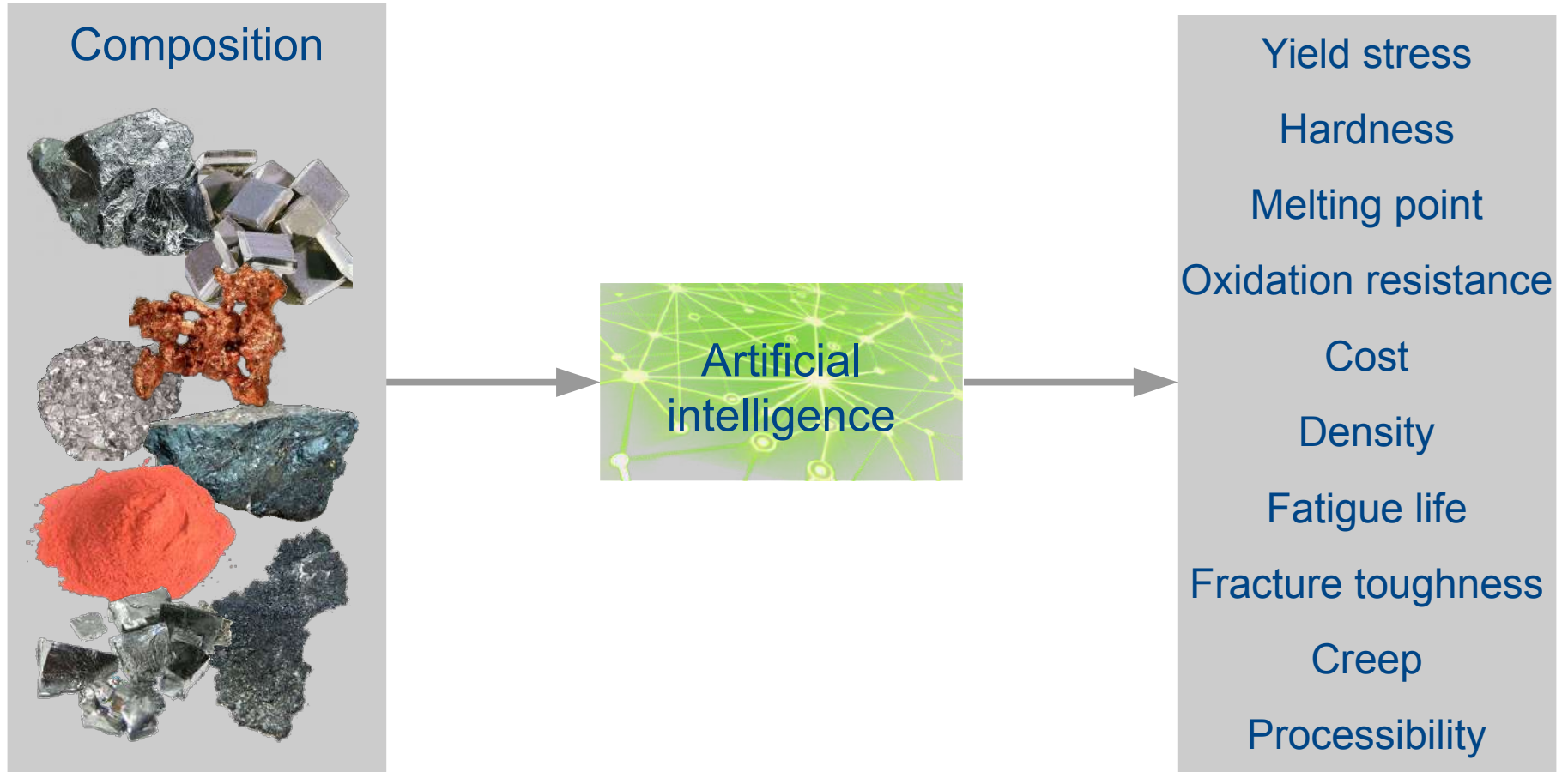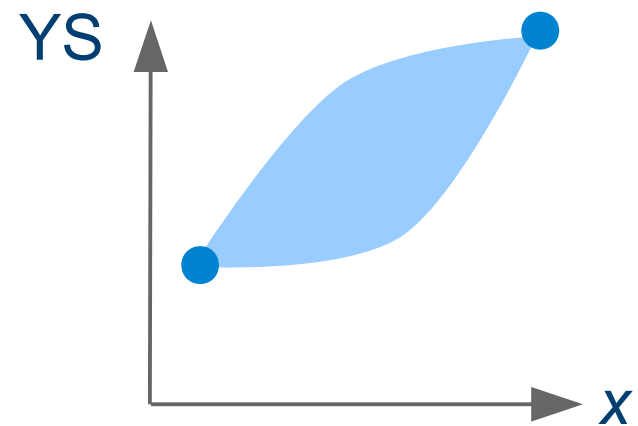**Mo-Hf forging alloy**
EP14161255
US 2014/223465

Mo-Nb forging alloy
EP14161529
US 2014/224885

Artificial intelligence
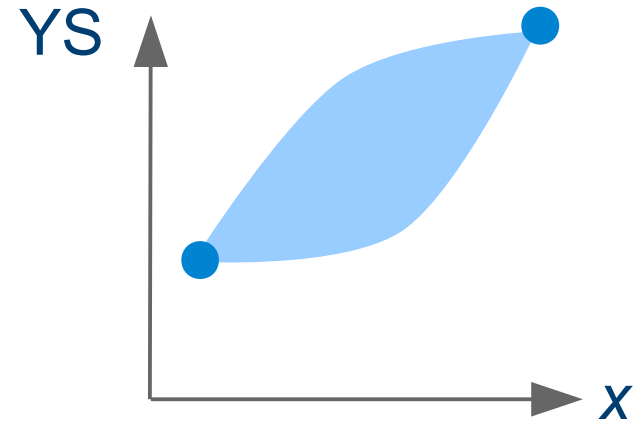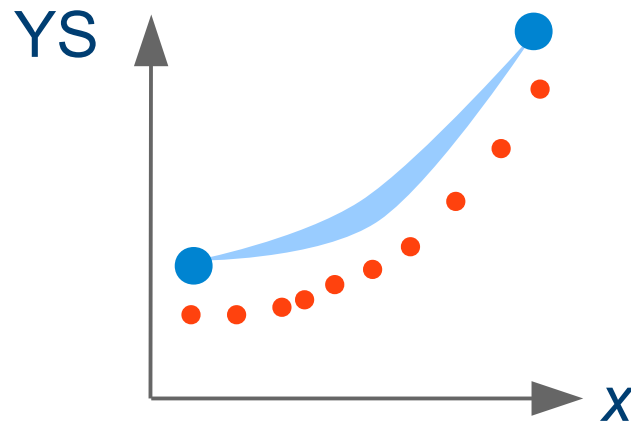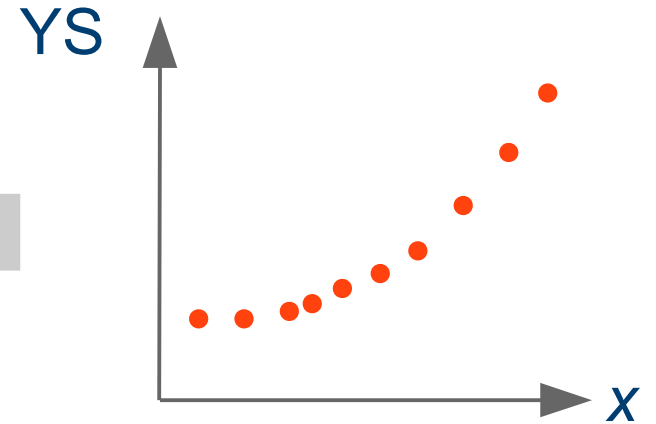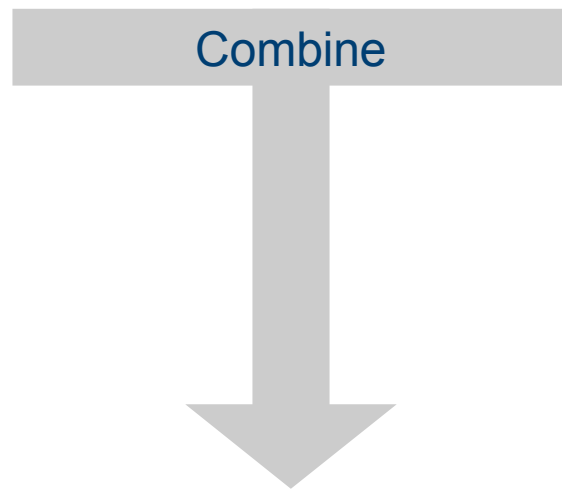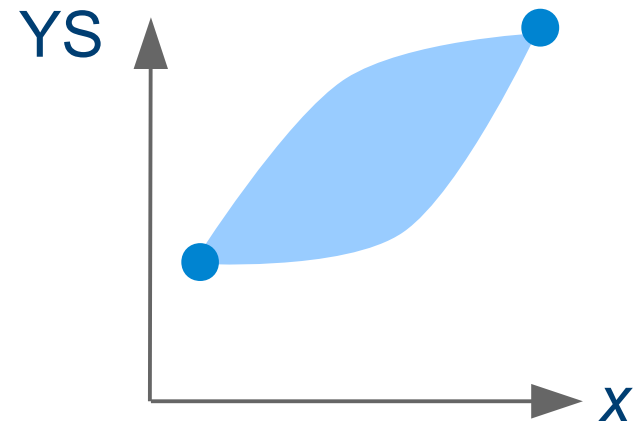
Merging simulation and experiment

Merging simulation and experiment
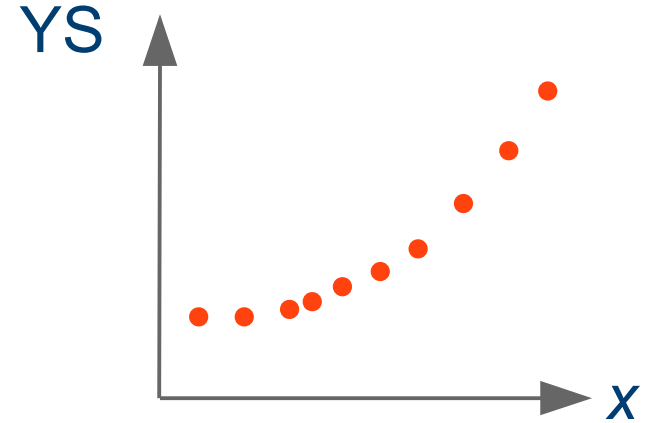
Merging simulation and experiment

Exploiting experiment and simulations

Lithium cathode materials

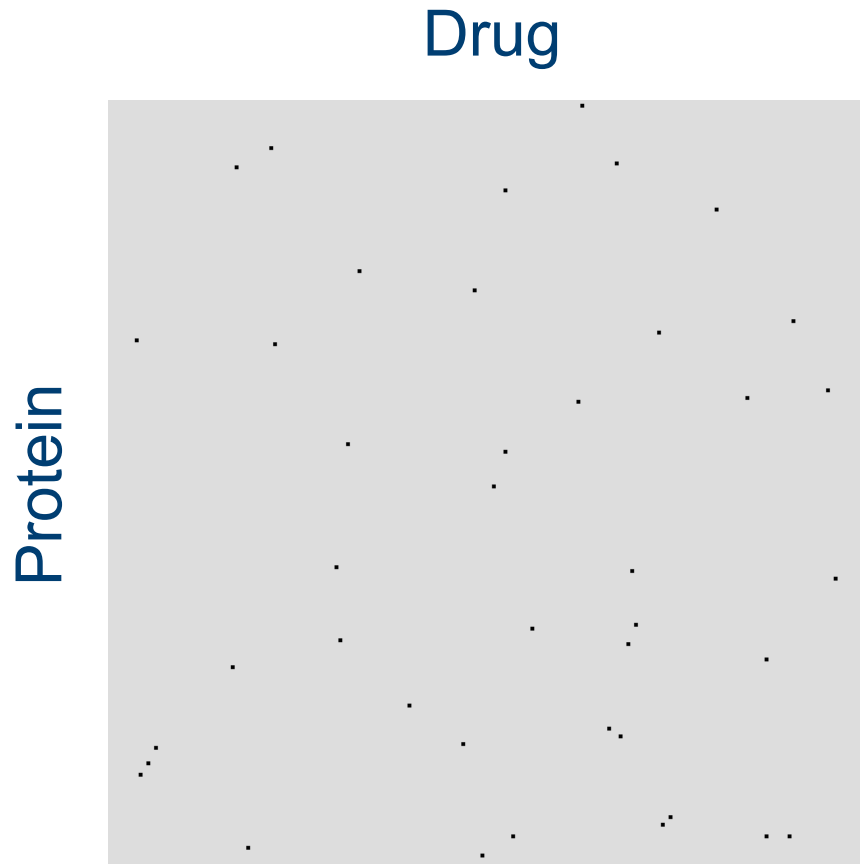| Experiment	DFT

Database verification
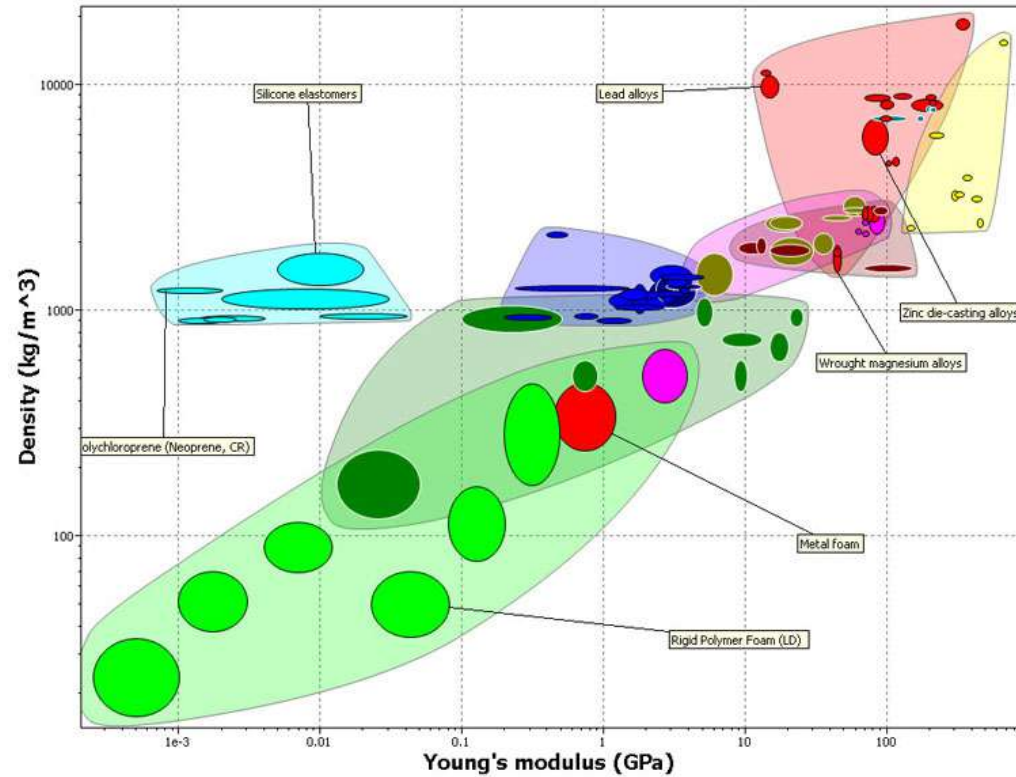
Found 156 erroneous points confirmed against primary sources
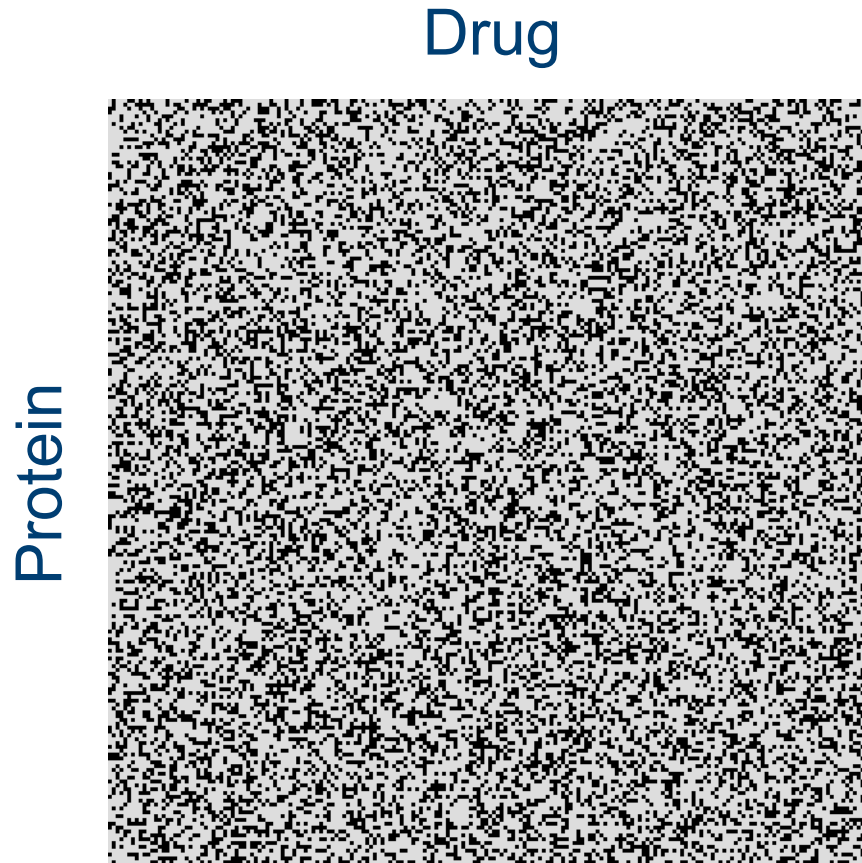
Protein activity data

ChEMBL database has protein activity for 0.1% of compounds

Drug

Protein

Protein activity data

Filled in 32% of the data points with 99.3% accuracy

Drug

Protein

Summary

Used artificial intelligence to discover materials

Can handle fragmented data

Merge simulations and experiments into holistic design tool

Proposed four new alloys, experimentally verified