Deep learning in materials design and drug discovery

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Neural network algorithm to

Merge all possible sources of information

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

Crystal structure
Neural network: train on complete data

Materials design

Materials design
Neural network: train on complete data

Crystal structure → [Image] → Crystal structure
Neural network trains on fragmented data
Neural network predicts on fragmented data
Materials: experimental interlude
Materials: experimental interlude
Schematic of an engine
Proposed alloy

Cr: 15.8  Co: 20.0  Mo: 0.5  W: 0.5  Ta: 4.9  Nb: 1.1  Al: 2.4

Ni: 47.2  Ti: 3.0  Fe: 3.9  Mn: 0.2  Si: 0.2  C: 0.02  B: 0.06  Zr: 0.18

900°C  30 hours
Predict the yield stress

![Graph showing yield stress vs temperature]

Yield stress / MPa

Temperature / °C

Proposed theory
Test the yield stress

![Graph showing the yield stress as a function of temperature. The graph includes a line graph representing the proposed theory and data points labeled RR1000.]
Test the yield stress

Yield stress / MPa

Temperature / °C

Proposed theory
Proposed experiment
RR1000
More materials designed
Apply deep learning to high-value **fragmented** data

Merge all sources of information into a **holistic** design tool

Experimentally **proven** materials and drugs design

Steels demonstrator: [https://app.intellegens.ai/steel_search](https://app.intellegens.ai/steel_search)