



Intellegens

# Introduction to Intellegens at IDMBAT

## About

Machine learning software to aid experimental design

**Merge** and aggregate all sources of data: experimental, computational, and analytical

Predictive models **reduce costs** and **accelerate discovery** process

## Traditional experimental design

Process is **expert driven**, subjective, and **iterative** through trial and improvement

Process takes ~20 years and specialist alloys cost >\$10m to develop, drugs cost >\$1bn

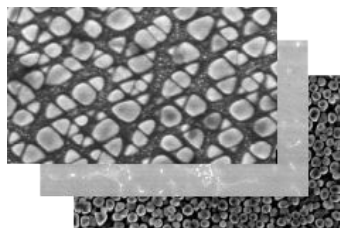
## Alchemite™ optimized design process

Alchemite™ predicts from **available** inputs: **property-property** correlations and computer simulations

**Reduce costs** - 90% reduction in experiments and fewer measurements for expensive quantities

**Accelerate** discovery and validation to 2 years

# Materials designed



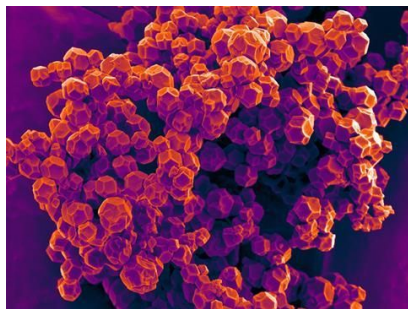
Nickel & moly alloys



Batteries



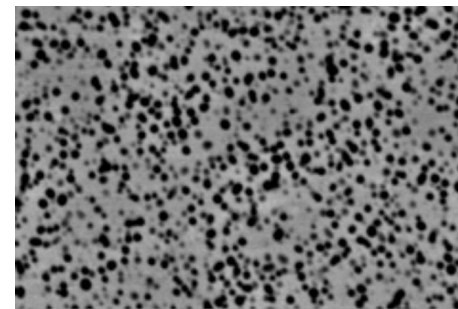
Steels of welding



Metal-organic framework

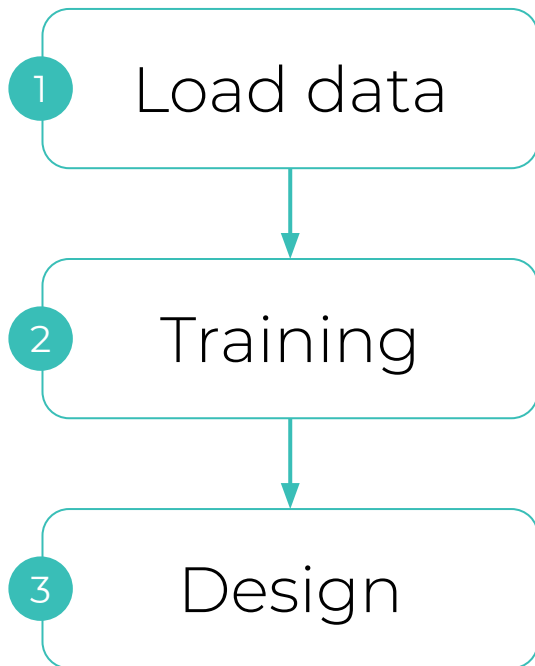


Concrete



3D printing

# Future opportunities: Integrated software



### Predicting properties of steel

We demonstrate a neural network that predicts the physical properties of steels based on the composition and heat treatment. The neural network model was trained from a library of experimental data from 1000 alloys.


In the first panel below set the percentages of each element in the composition and heat treatment temperature, and then click predict to get the neural network estimates for yield stress, ultimate tensile strength, and elongation.

Click [here](#) to use this technology to optimize the yield stress, ultimate tensile strength, and elongation the steel.

This same technology was used to understand nickel alloys where the composition covered 20 elements, 5 heat treatment parameters, and predicted 11 material properties. Click here to read more about this study.

Click here to optimize a composition for given targets

Set inputs		
Iron (Fe)	<input type="text" value="100"/>	remain %
Carbon (C)	<input type="text" value="0"/>	0 to 0.43 %
Manganese (Mn)	<input type="text" value="0"/>	0 to 3.0 %
Silicon (Si)	<input type="text" value="0"/>	0 to 4.75 %
Chromium (Cr)	<input type="text" value="0"/>	0 to 17.5 %
Nickel (Ni)	<input type="text" value="0"/>	0 to 21.0 %
Molybdenum (Mo)	<input type="text" value="0"/>	0 to 9.67 %
Vanadium (V)	<input type="text" value="0"/>	0 to 4.32 %

 PREDICT

Predictions	
Yield Stress (MPa)	1605 ± 46
Ultimate Tensile Strength (MPa)	1200 ± 67
Elongation (%)	9 ± 2

# Machine learning for materials design

**Merge** sparse databases to deliver deep insights into new materials

Designed and **experimentally verified** alloys, chemicals, and drugs

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Papers	<a href="https://www.intellegens.ai/paper.html">https://www.intellegens.ai/paper.html</a>