intellegens

DATA-DRIVEN DISCOVERY

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NOVEL APPROACH TO MATERIAL DESIGN USING DEEP LEARNING FOR SPARSE EXPERIMENTAL DATA

We have developed a unique deep learning toolset, Alchemite™, that can learn property-property relationships between all available parameters in sparse datasets that are as little as 0.05% complete. This novel algorithm is capable of combining limited amounts of high-quality experimental data with plentiful, but potentially lower-quality, computer simulation or public domain data. Through this combination, Alchemite™ can identify key features in the data and design new compositions to satisfy stringent property constraints.

NEW ALLOY FOR DIRECT LASER DEPOSITION

The Alchemite™ deep learning algorithm was used to design a new nickel-based alloy for direct laser deposition for use as a combustor within a gas turbine engine. The new superalloy had properties that exceeded those of other commercially available alloys.

SAVED 15 YEARS
OF RESEARCH

REDUCED DEVELOPMENT COSTS BY
$10 MILLION

A large weldability database was used to guide the extrapolation of the 3D printing relationships, which enabled the algorithm to capture new insights into the material properites and identify a new material and accompanying processing conditions of the best alloy for additive manufacturing.

OPTIMISING ALKANE PROPERTIES FOR LUBRICANTS

By combining sparse experimental data with molecular dynamics simulations to predict physical properties of alkanes, Alchemite™ sped up the identification of alkanes to be used for lubricant base oils with superior physical properties.

10x FASTER
IDENTIFICATION OF ALKANES

5x MORE ACCURATE
ESTIMATION OF INTRACTABLE PROPERTIES

Alchemite™ accurately estimated intractable properties including density and shear viscosity and produced results that were more accurate and consistent than those reproduced by other methods.

CURRENT APPLICATIONS

- Design of Alloys, Superalloys, Composites, Plastics, Polymers, Plastics, Glass, Rubber
- Chemicals
- Batteries
- Predictive Maintenance
- Process Optimisation
- Drug Discovery
- Food & Beverage
- Cosmetics
- Exploration and optimisation of oil and gas sites

PAPERS

1. Ng, M. et al. (2020). Predicting the state of charge & health of batteries using data-driven machine learning. *Nature Machine Intelligence*. Manuscript accepted for publication.
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3. Santak, P. & Conduit, G. (2019). Predicting physical properties of alkanes with neural networks. *Fluid Phase Equilibria, 501*, 112259.
4. Moghadam, P.Z. et al. (2019). Structure–Mechanical Stability Relations of Metal-Organic Frameworks via Machine Learning. *Matter, 1*, 219.
5. Conduit, B.D. et al. (2018). Probabilistic design of a molybdenum-base alloy using a neural network. *Scripta Materialia, 146*, 82.