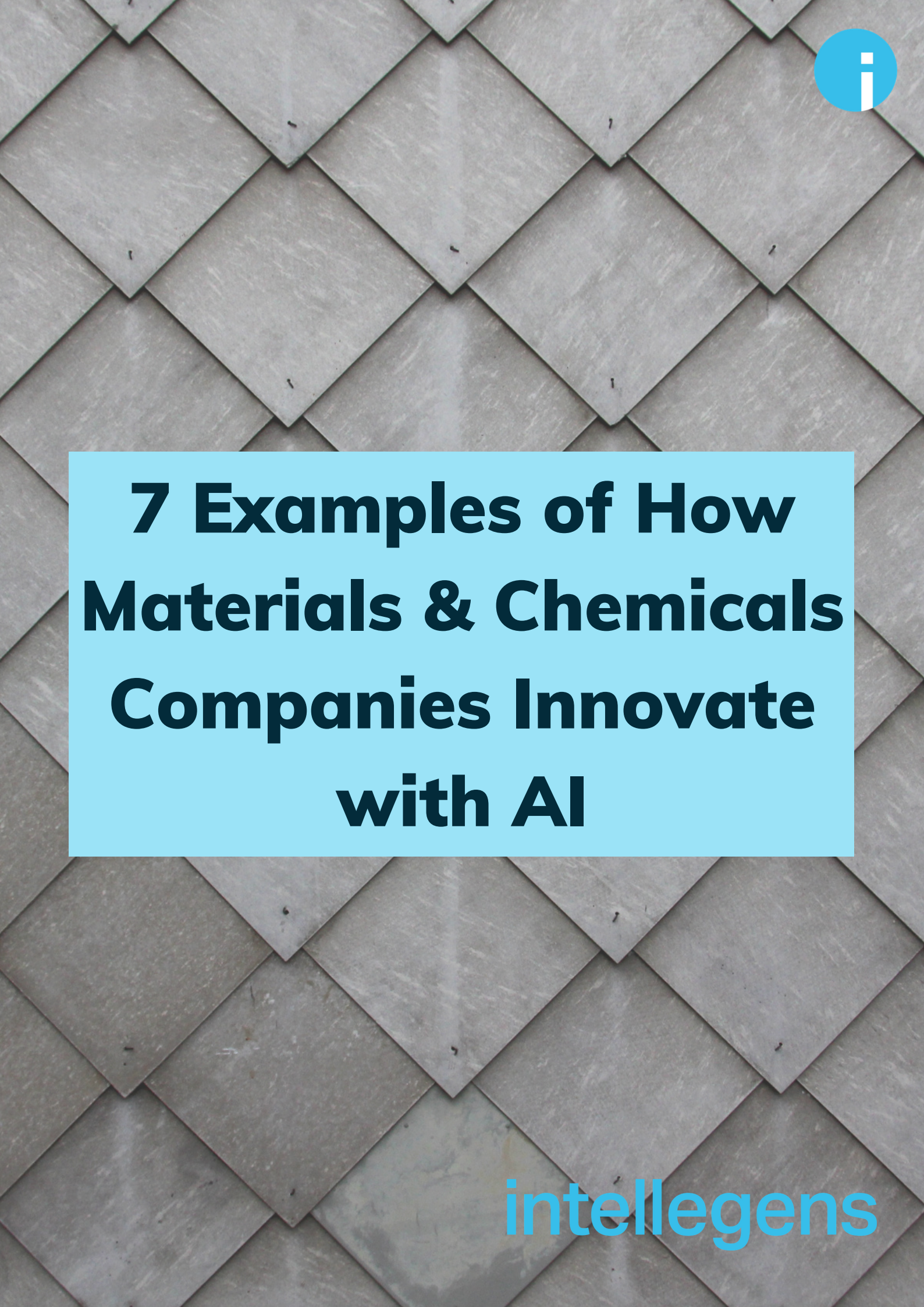


7 Examples of How Materials & Chemicals Companies Innovate with AI

intellegens

Case Studies

We present 7 ways materials and chemicals companies adopted machine learning to accelerate R&D and shorten the time to market.

High-Performance Alloys for Aerospace

Design of a nickel-base alloy for a jet engine using machine learning.

Batteries

Predicted state of health, state of charge, and designed the best possible chemical characteristics of molecules that can prove to be the basis of a next-generation battery material.

Forging Hammers

New molybdenum-base alloys found with 5-fold reduction in experimental time and cost.

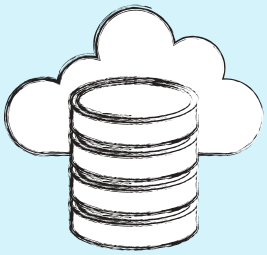
Antimalarial Drug Discovery

Built accurate predictive models for activity against the target.

Optibrium & Open Source Malaria initiative

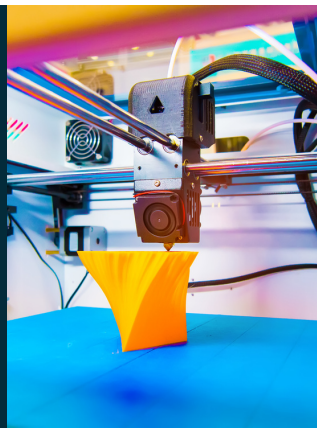
Data Validation

Implemented a fast way to automatically validate complex numerical data.



3D Printing

Combined historical data with sparse data to optimize this additive manufacturing process saving 15 years of research.



Alkanes for lubricants with superior physical properties

Accurately estimated intractable properties and produced results that were more consistent than those reproduced by other methods.

High-Performance Alloys for Aerospace

Challenge

Commercially available superalloys are the outcome of several years of empirical research and development. Even though these superalloys have good properties, they do not necessarily have the optimal balance of properties required for specific engineering applications.

Solution

Computational design tool, Alchemite™, incorporates uncertainty to allow alloys to be designed with the greatest probability of meeting a design specification containing many different material properties. Alchemite™ combines experimental data with computational thermodynamic predictions to rapidly, reliably, and robustly identify the alloy composition that is most likely to meet a multi-criterion specification.

Alchemite™ was used to propose a new nickel-base superalloy most likely to simultaneously fulfill 11 different physical criteria.

Outcome

Alchemite™predicted that the new nickel-base alloy offered an ideal compromise between its properties for disc applications and seven of these properties were experimentally verified, demonstrating that it has better yield stress and oxidation resistance than commercially available alternatives. The capability to quickly discover materials computationally using Alchemite™ empowered engineers to rapidly optimize bespoke materials for a specific applications, bringing materials into the heart of the design process. Alchemite™ has also been used to design a nickel-base alloy for a combustor liner, and two Mo-based alloys for forging tools.

Paper

B.D. Conduit, N.G. Jones, H.J. Stone, G.J. Conduit (2017). Design of a nickel-base superalloy using a neural network. *Materials & Design, 131*, 358-365.

Reduced development costs by £10m

https://intellegens.ai/materials/aerospace/

Batteries

Challenge

The performance, cost and safety of batteries determine the successful development of electric vehicles (EVs). Further research of battery chemistries will result in more complicated battery dynamics, where safety and efficiency will become a concern. Therefore, an advanced battery management system (BMS) that can optimize and monitor safety is crucial for the electrification of vehicles.

Solution

Machine learning to design the cathode, anode, and electrolyte and predictive models for battery management systems to alleviate range anxiety. Alchemite's™ predictive models standardize processes and reduce costs both in terms of the number of experiments that need to be performed and optimizing experiments to minimize the need for expensive components or processes.

AI manages state of health and charge, predicts remaining useful life, and reduces the number of prototypes needed in testing.

Outcome

Our deep learning technology ran virtual experiments to focus the search for new materials. Alchemite™ predicted remaining useful life, state of health and state of charge while reducing fabrication and development costs and improving key battery metrics for process parameter prediction.

Press Release

Data-driven machine learning is the best approach for advanced battery modelling

Paper

Man-Fai Ng, Jin Zhao, Qingyu Yan, Gareth J. Conduit, Zhi Wei Seh (2020). Predicting the State of Charge and Health of Batteries using Data-Driven Machine Learning. *Nature Machine Intelligence, 2,* 161-170. *https://doi.org/10.1038/s42256-020-0156-7*

Forging Hammers

Challenge

Forging hammers wear and degrade through repeated use, can they be made more durable? Machine learning is capable of exploring new alloys to improve strength at elevated temperatures.

Solution

Augment experimental data with thermodynamic models that incorporate uncertainty to propose molybdenum-base alloys with the highest likelihood to meet design targets. Alchemite™ is able to suggest new precipitate chemistry with improved properties.

5-fold reduction in experimental time and cost

Outcome

New molybdenum-base alloys were found with 5-fold reduction in experimental time and cost. Our technology improved molybdenum-base hammers lifetime by 30%, reducing both deployment costs and factory downtime.

Paper

Conduit, B.D., Jones, N.D., Stone, H.J., Conduit, G.J. (2018). Probabilistic design of a molybdenum-base alloy using a neural network, *Scripta Materialia,146*, 82-86. https://doi.org/10.1016/j.scriptamat.2017.11.008

Antimalarial Drug Discovery

Challenge

Identify a new antimalarial compound against a novel antimalarial mechanism of action. Over the past six years, the Open Source Malaria (OSM) project has brought together an international team of researchers who design, synthesise and test new antimalarial candidates that they hope will demonstrate potent activity against Plasmodium falciparum, the deadliest species of the malaria-causing parasite, in vitro and in vivo. However, the available bioactivity data is sparse; for all of the assay endpoints that are available, only a very small proportion of the compounds have actually been measured.

Solution

Alchemite™ is able to predict the activity of compounds against a novel mechanism of action and has shown to significantly improve the accuracy of the predictions and outperformed conventional quantitative structure-activity relationship (QSAR) and other AI models in a blind test conducted by OSM. Alchemite™ accurately predicted activity of compounds against a novel mechanisms of action.

Accurate prediction by Alchemite™ prioritises high-quality compounds, reducing research and development costs associated with unnecessary synthesis and testing.

Outcome

Alchemite™ was applied to novel compounds generated automatically by Optibrium's StarDrop™ software. A compound that was confidently predicted to be active was proposed by Intellegens and Optibrium for synthesis and testing by OSM. Out of the compounds proposed by four organisations, only our entry demonstrated potency against the target. The measured activity was in strong agreement with the predicted values. The predictive accuracy of Alchemite™ outperforms the leading approaches.

Press release

Optibrium and Intellegens achieve further success in Open Source Malaria initiative with in vitro validation of in silico generated compound

Paper

T. M. Whitehead, B. W. J. Irwin, P. Hunt, M. D. Segall, and G. J. Conduit (2019). Imputation of Assay Bioactivity Data Using Deep Learning. *Journal of Chemical Information and Modeling, 59*(3), 1197-1204. DOI: 10.1021/acs.jcim.8b00768

For more information, visit https://www.optibrium.com/augmentedchemistry

https://intellegens.ai/drug-discovery/small-molecule/

Data Validation

Challenge

Recording complex experimental data is critical if it is to be trusted in the future. Companies that sell curated databases must have efficiently identified and fixed all erroneous entries. Errors in central database misguides research programs and will lead to inaccurate machine learning.

Solution

Alchemite™ was used to generate machine learning models from the entire data corpus, skipping over any missing data and taking into account standard noise in any of the measurements. The resulting model was then used to re-predict several million data points in the corpus, giving a set of predicted values. The predicted values were then compared to the given values and using the confidence in the predictions enabled us to identify outliers that warranted manual inspection.

Outcome

Alchemite™'s deep learning algorithms automatically validated an entire experimental corpus, with no explicit domain knowledge, learning expected correlations between all available data and identifying data points that were not consistent with the model. We identified a range of outliers which were typos, experimental errors, or genuine outliers - giving the client a cheap, fast way to automatically validate complex numerical data. Our technology increased the confidence and breadth of results generated dramatically.

https://intellegens.ai/software-data/data-validation/

Alkanes for Lubricants with Superior Physical Properties

Challenge

Lubricants need to be optimized for new applications such as electric vehicles. Given that lubricants are mixtures of predominantly alkanes, it is unclear whether contemporary lubricant formulations are the most optimal. Lubricants contain hydrocarbon molecules, therefore predicting the properties of hydrocarbons facilitates the development of base oils.

Solution

Deep learning algorithm Alchemite™ can exploit property-property correlations to predict the physical properties of alkanes. Alchemite™ inputs the molecular structure of alkanes to predict the boiling point, heat capacity, and vapor pressure as a function of temperature. The results reproduced by this algorithm are significantly more accurate and consistent than those reproduced by other methods.

Outcome

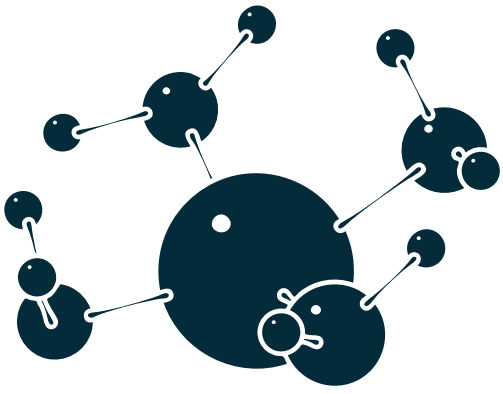
By combining sparse experimental data with molecular dynamics simulations to predict physical properties of alkanes, Alchemite™ accelerated the identification of optimal hydrocarbons tenfold. Alchemite™ also accurately estimated intractable properties including density and shear viscosity and produced results that were five times more accurate and consistent than those reproduced by other methods.

Press release

Deep Learning Tool Enables the Identification of Alkanes For Lubricants With Superior Physical Properties

Paper

Santak, P. & Conduit, G. (2019). Predicting physical properties of alkanes with neural networks. *Fluid Phase Equilibria, 501*, 112259.



10x faster identification of alkanes

https://intellegens.ai/chemicals/lubricants/

3D Printing

Challenge

Additive Manufacturing (AM) is a new processing technology used in a wide range of industries to produce and repair bespoke and high-value parts including, for example, aerospace engine components, turbine blades, and oil drilling tools. To date, very few materials have been fully experimentally verified going through these processes, severely restricting the application of the technology to wider fields of use. A particular challenge is that the ability to print materials is poorly understood - direct laser deposition (one AM method) has only been applied to just ten sets of processing variables. This provides a mere ten data points which are not enough for traditional machine learning techniques to predict the properties of a wider family of processing variables.

Solution

We optimized the direct laser deposition process for AM using historical welding data and the available sparse direct laser deposition dataset. Alchemite™ was able to leverage abundant weldability data to automatically identify and exploit property-property relationships enabling the capture of new insights into the changing processing variables.

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 properties.

Outcome

By using historical welding data combined with the sparse data from direct laser deposition, we were able to optimize this AM process and broaden its application to new processing variables, saving 15 years of research. Quicker than conventional production techniques, AM has the potential to save manufacturers vast amounts of time and money. This approach is not limited to AM and can be applied to the introduction to any manufacturing process.

Saved 15 years of research

Paper

B.D. Conduit, T. Illston, S. Baker, D. Vadegadde Duggappa, S. Harding, H.J. Stone & G.J. Conduit (2019). Probabilistic neural network identification of an alloy for direct laser deposition. *Materials & Design* ,*168*, 107644.

https://intellegens.ai/materials/additive-manufacturing/

About Intellegens

Intellegens has developed a unique artificial intelligence engine, Alchemite™ for training neural networks from incomplete, sparse, and noisy data, typical of real-world data. The technique was first developed at the University of Cambridge where it has been used to develop several superalloys, guide the design of new drugs and help optimise battery pack design. The tool is now being used to solve a wide range of real world industrial process problems where rare but valuable data can be used to improve real world industrial processes leading to reduced costs and environmental impact.

For more information, visit intellegens.ai.

For more information on the **Alchemite™ Analytics platform** vist https://intellegens.ai/alchemite-analytics/

Want to learn more about how our AI technology can be applied to your specific needs? Contact us to learn more at info@intellegens.ai

Click on the link below to subscribe to our latest news and upcoming events

https://intellegens.ai/subscribe

intellegens

intellegens.ai
info@intellegens.ai
@intellegensai