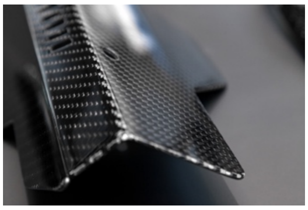
WHITE PAPER

Trustworthy AI in the materials and chemicals industries

A feasibility study on accelerating adoption of machine learning in support of innovation

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Applied machine learning

Executive Summary

This white paper reports the results of a project supported by **Innovate UK** and involving a Consortium of industry and academic partners coordinated by **Intellegens**, to identify **factors limiting the adoption of AI in the chemicals and materials sectors**, particularly in R&D and process optimisation. The aim of the study is to guide future work, at both an industry and organisational level, to enable more effective application of AI technologies, particularly **machine learning (ML)**. This work is motivated by the strategic importance of these industries, which are worth over £74bn to the UK economy and over $5 trillion globally, and the potential of AI to tackle key challenges for the sector. These include accelerating innovation, responding in an agile manner to price and supply chain volatility, navigating complex regulatory environments, and achieving net zero and sustainability goals.

We have found **strong industry interest in adopting AI/ML technologies**, particularly, initially, in R&D. Many organisations have made a good start, often with positive outcomes. We could identify many **case studies** of successful use and have shared some in this paper. Those that are yet to implement AI/ML at all in areas such as design of experiments are certainly behind the curve. But we have also found plenty of **scope to widen, deepen, and accelerate this implementation** in every organisation studied, with current projects often confined to expert project teams or a small number of pilot projects. We identified some of the **key issues that might act as a brake on adoption**. These included issues of **organisational culture**, concerns about the **transparency** of the technology, and the state of **data management** and **integration** with other information technologies.

We conclude that a **step-change in the application of machine learning** to support innovation in the industries studied is both desirable and achievable – indeed, it is inevitable. This will primarily be driven by individual research organisations making smart return on investment decisions informed by growing evidence of the value of the technology. But **this process can be accelerated and facilitated** by proactive steps to mitigate organisational and cultural barriers to adoption, by industry-level education initiatives, and by commercial software and service vendors optimising their offerings. We have suggested some areas on which to focus future efforts – both industry-wide, for individual chemicals and materials organisations, and for vendors. More detailed analysis and action in these areas might be the focus for future industry collaboration.

Background

The materials and chemicals industries

The materials and chemicals market in the UK is a significant part of the country's economy, with chemicals industry revenues alone valued at £74 billion in 2020 [1]. The market offers diverse products including basic and specialty chemicals, agrochemicals, personal care products, alloys, plastics, and advanced materials. The global market is worth over $5 trillion and is expected to grow over the next 5 years at an estimated compound annual growth rate (CAGR) around 4-5% [2]. This growth will be driven by increasing demand for materials and chemicals in construction, transportation, and consumer goods. Adoption of new technologies such as electric vehicles and renewable energy will also boost growth. That materials and chemicals organisations are essential suppliers to such industries emphasises their strategic importance.

Materials and chemicals are a large and strategic part of the UK and global economies

Key challenges for the industry are:

- **Accelerating innovation:** competitive pressures are high [3], with limited scope to compete on price in a globalised commodity market for many participants. Differentiation is through superior and specialised products and expertise, requiring a ‘conveyor belt’ of innovations that brings new products to market as fast as possible.
- **Price and supply chain volatility:** The supply chain for the chemicals industry is huge, complex, and volatile [4]. It is subject to geopolitical events, changing regulations, and large movements in the prices of raw materials. The industry needs to maintain agility to respond to these changes while operating at scale.
- **Regulations:** As well as impacting the supply chain, regulations designed to protect human health and the environment add challenges to product and process development [e.g., 5]. Companies may need, for example, to rapidly find substitutes for a key ingredient that has been rendered obsolete or to change a critical process step.
- **Net zero and sustainability:** All major players in the industry are setting tough goals to lower their energy consumption and carbon footprint and remove waste from their processes [6]. Including these additional objectives complicates the task of optimising the processing and applicaton of materials and chemicals.

Such challenges place increased pressure on R&D and manufacturing teams to achieve project goals faster and to squeeze every drop of performance from products and processes. This in turn is driving greater interest in AI technologies to maximise value from legacy data, find optimal experimental and process routes, and make smart real-time process decisions.

These strategic challenges are driving greater interest in AI

The potential impact of AI

The Artificial Intelligence (AI) market in the UK was itself valued at £7.5bn in 2021 and projected to reach £11.7bn by 2025 [1]. This reflects both UK strengths in AI technologies such as machine learning (ML) and growing adoption across sectors such as healthcare, finance, retail, and transportation. In the chemicals sector, 80% of executives surveyed in a recent IBM report [7] said AI would be important to business success in the following three years. Some key focuses included:

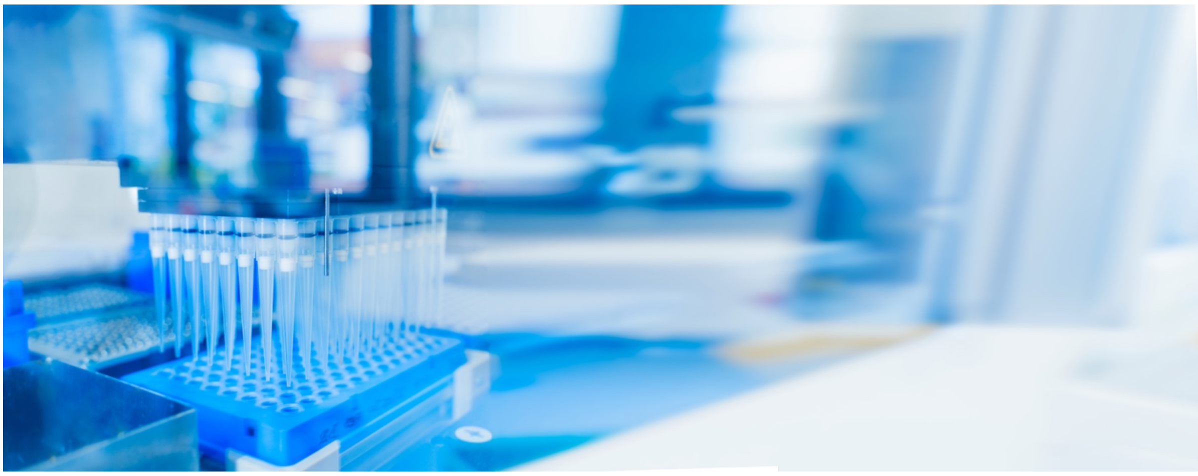
80% of chemicals industry execs said AI would be important to business success in the 3 years after 2020

- Design of experiments
- Discovery of new materials
- Product portfolio optimisation
- Feedstock optimisation and load forecasting of new materials
- Process management and control

Just 25% of chemicals companies had implemented AI for design of experiments

At Intellegens, where our focus is largely on the R&D function, we have reported examples of using machine learning to achieve measurable reductions in experimental costs, improved yields in chemical processes, and new insights into the mechanisms determining key product properties (more details below).

Yet, even within the R&D domain, the IBM report found just 25% of organisations had so far implemented AI for design of experiments. Our own experience is that, within these organisations, usage of AI-based methods is often restricted to data scientists or enthusiasts within the wider scientific team. Machine learning is far from a routine tool on the desktop of every scientist. This is despite the fact that the IBM report also identified R&D as the area in which AI implementations were most common in the chemicals industry, ahead of functions such as manufacturing and materials sourcing.



The focus of this project and report

This white paper describes '**Trustworthy AI for the materials and chemicals industries**', a project that aimed to address this situation by understanding some of the reasons constraining the use of AI, and in particular ML, in these industries. It focused on usage in R&D as the pioneering function in the roll-out of AI technologies, while considering implications for other functions, such as production. Led by Intellegens, the project was sponsored by Innovate UK KTN, part of UK Research and Innovation, as part of a wider "Accelerating trustworthy AI" funding initiative [8] from the UK Government that aims to drive greater impact for AI in strategic industries. Intellegens assembled a consortium of industry and academic partners from the materials and chemicals sector with the initial aim of producing a feasibility study and guidance for further work that might support wider adoption.

Methodology

Consortium

The key vehicle for the 'Trustworthy AI' project was a Consortium of industry and academic organisations with interests in materials and chemicals.

Organisation	Relevance
Johnson Matthey	Chemicals industry leader in sustainable technologies
Goodfellow	Leading global supplier of materials for R&D
Domino Printing Sciences	Develop advanced ink formulations
Welding Alloys Group	Develop materials and hardware for welding applications
Henry Royce Institute	The UK's national institute for materials research
University of Cambridge	Novel machine learning methods for physics and materials
University of Leicester	Applications of AI in metallurgy
Intellegens	Applied machine learning software provider

Process

The Consortium held a series of interviews with members and group discussion sessions in the Spring of 2023, including a face-to-face seminar on the Genome Campus near Cambridge in May. These identified key barriers to adoption for AI/ML in the experience of member organisations, both from within their own organisations and from their interactions with colleagues in other organisations. This discussion was informed by a survey that was distributed among Consortium members and their wider network. Having identified key themes among the barriers to adoption, members shared best practices and ideas designed to overcome them. These were captured and summarised by the project team, supporting a final discussion in which areas for future action were identified.

Findings

Positive case studies, but slow progress

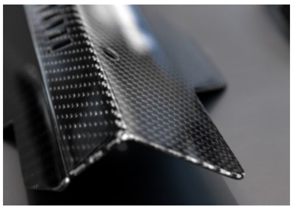
83% had adopted ML in some form, but often this was still at pilot project stage

Our discussions and survey process validated the landscape introduced above, including in the IBM report. Of the organisations touched, we found that 83% had adopted AI/ML in some form that was linked to ongoing strategic objectives. We note, however, that the sample is biased towards organisations interested in discussing the future of AI/ML in the industry. Our conclusion is thus that this observation supports the assumption of widespread interest in the technology, but not yet universal adoption. More notably, the minority within these organisations reported that adoption was not widespread within their businesses, with the current focus in most on piloting AI/ML in one or more business areas.

Members were able to report case studies of successful applications. Examples include:

- Extracting insight from experimental data to enable re-formulation of inks in response to changing regulations. [9]
- Finding process changes that increased the yield of a key production processes in manufacturing a catalyst. [10]
- Identifying experimental routes that could cut the amount of experiment needed to develop a process by 50-80%. [11]
- Designing a new surface treatment to improve the wear performance of an alloy. [12]






The most significant benefits are in accelerating R&D and process optimisation

In general, participants saw the most significant benefits from AI/ML today as being in accelerating R&D and in process optimisation. In most cases, however, these successful use-cases resulted from a small group of interested researchers acting as an 'expert AI/ML team' within the organisation, often with scientific support from an external AI/ML provider such as Intellegens. They typically found projects to which the technology could be applied in 'consultant mode'. This contrasts with a model where the AI/ML is an integrated tool within the workflow of scientists that is routinely applied to data analysis in every project. Some of the organisations interviewed were taking steps to encourage increased adoption and saw this as a strategic objective.

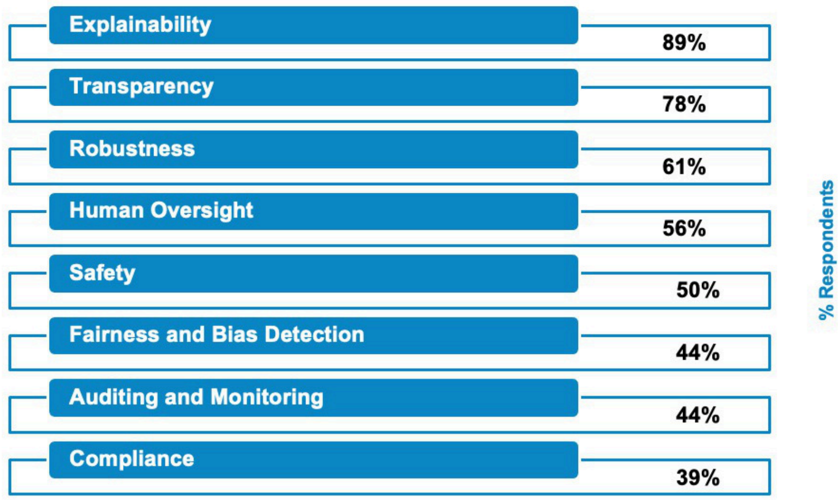
One interesting issue was whether, in organisations where teams had developed expertise in applying AI/ML, the personnel involved were data scientists who had become sufficiently familiar with the chemistry/materials problems being studied, or physical scientists who had learned enough about AI/ML. In fact, we found examples of both, supporting the idea that wider adoption among chemists and materials scientists is a valid objective.

Barriers to adoption

Our project members and survey responses identified those factors that they felt were most significant in slowing the adoption of AI/ML in the chemicals industry. Key factors were.

1. **Resistance to change / inertia.** Our survey indicated resistance to change as the primary bottleneck for adoption (often described as "inertia" during interviews). This finding, also reflected in a 2020 study by McKinsey [13] into factors resulting in underutilisation of AI capabilities, is unsurprising. Such inertia is often cited as a key issue in the deployment of any new technology. Teams are preoccupied with existing tasks and do not feel that they have time or space to consider new approaches or to implement change effectively. Team leaders may feel current approaches are "good enough" – already yielding satisfactory results while under pressure to deliver. Our interviews identified that often technical teams are keen to use new technologies, but managers have concerns about disruption to productivity or want more hard evidence of the efficacy of new approaches. IT or legal requirements for adopting new tools (e.g., security compliance for software systems or questions about intellectual property relating to ML models) add to the effort involved, increasing reluctance.

2. **Trustworthy AI.** A collection of issues that can be grouped under this heading was the next most prevalent factor. These are explored in more detail in the next section. They include anything that raises concerns among scientists or their managers that the technology may lack transparency (meaning they would be unable to fully inspect or justify the logic behind decisions) or may include hidden biases or assumptions.



Key 'Trustworthy AI' factors as identified by survey participants – further discussion in the next section.

3. **Data quality and standardisation**. Datasets are often highly heterogeneous and inconsistently structured, particularly when integrating data from different sources. Respondents' feedback indicated that lack of good data management and stewardship such as, for example, standard data formats and effective metadata management, pose challenges in integrating diverse data sources for AI/ML model development and deployment. There was often an unwillingness to proceed with AI/ML analysis until a robust data management process was in place, even when using such analysis early could help organisations to understand their data better and thus to design more efficient data management structures. Related to this challenge is the fact that, as a Citrine report [14] highlights, materials and chemical datasets are often small (l00+ rows in a data rich scenario) and incomplete due to the cost and time of acquiring experimental data. Many ML approaches do not work well with small and/or sparse datasets.

4. **Integration of software systems.** The chemical and materials industries already use a wide variety of commercial software systems and in-house bespoke software, creating a diverse and complex scientific IT landscape. Tools often fail to use common standards, complicating the integration of any new technology with existing data and workflows. If the introduction of AI/ML requires use of new software, then the overhead involved in fitting it into this landscape can be a deterrent to its use. Strategies to overcome this challenge are varied. Some organisations advocate a move towards integrated platforms, with most tools provided by a single vendor or its partner ecosystem. Others (and this was the preferred model among our project members) prefer to find the best point solutions, provided that these use open, standard technologies that enable them to be connected to other systems. Whatever approach is adopted, this is an issue that both providers and users of AI/ML tools need to consider carefully.

5. **Organisational culture.** Closely linked to the first point above, some respondents identified the impact of organisational issues in slowing adoption. Issues cited included political factors, fear of failure, confusion, and ineffective delegation.

What is needed for trusted and responsible AI?

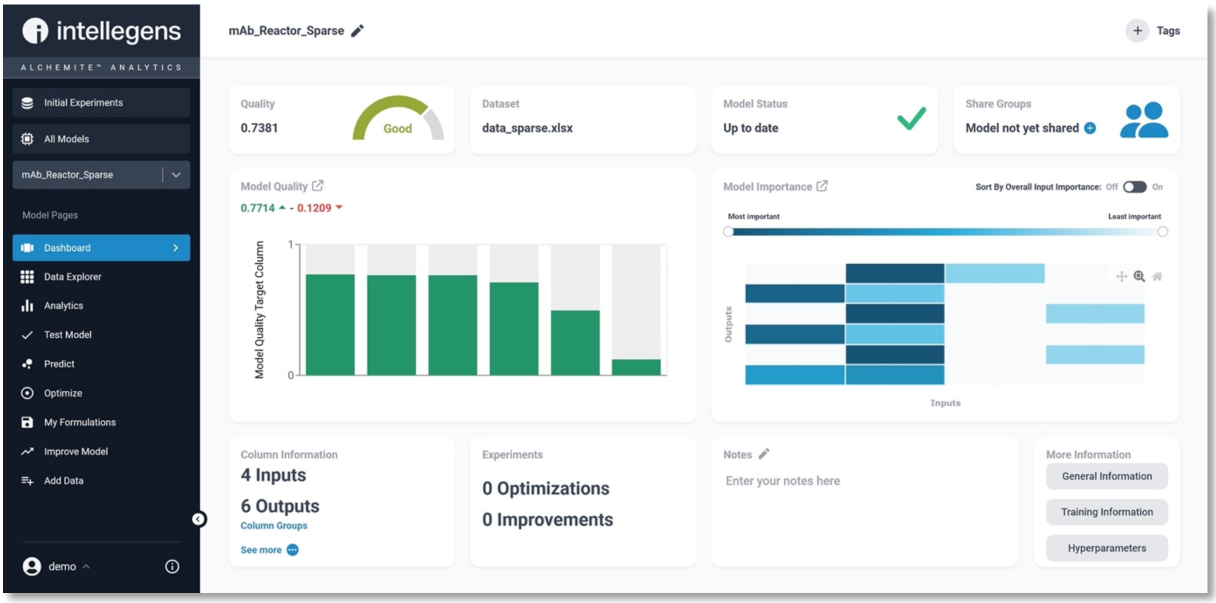
This section expands on the second item identified above: 'Trustworthy AI'. This was the main barrier to adoption that is specific to the technology, as opposed to a characteristic of the adopting organisation. Our research indicates that trust in AI systems varies depending on the user's background and expertise. Data engineers may seek additional information about the model before trusting its results, while users without a data science background, such as chemists and materials scientists, are more likely to accept answers from models if they appear appropriate and provide desired outcomes.

The pivotal issue is **transparency**. Understanding in-depth every detail of how an ML model works is usually impossible, given that the point of these models is typically to capture incomprehensibly complex non-linear relationships in multiple dimensions. But users do want to be able to inspect the decisions suggested, develop an understanding of the key relationships that the model is identifying, and review potential biases.

Users want to be able to inspect the decisions suggested by the ML model

Numerous studies have discussed this transparency [15], seeking a stronger connection between users and AI models. Some studies have even proposed measures to quantify the level of transparency in AI methodologies [16]. Others focused on the need to enhance user education, or the application of approaches like reverse reinforcement learning. But such publications tend to focus primarily on AI researchers and may not fully represent the perspectives of less specialist users.

Understanding the needs of these **'non data scientist' users** is crucial for establishing trust. Many seek validation from AI systems. If the suggested answers appear acceptable and align with their expectations, they are more likely to trust the results. A study [17] supports the idea that general audit and validation can foster trust, especially when users observe consistent results. To address situations where users lack trust, focus should be placed on improving result '**explainability**'. Interviews also exposed that disclosing uncertainties in the outcomes, and possibly even the method of uncertainty calculation, can help users to understand the limitations and decisions of the AI system, leading to a more trusted model.



An example machine learning tool, Alchemite™ from Intellegens, showing 'explainable AI' functionality that enables uses to understand model quality and inspect the relationships driving the ML model that the software has built.

The balance between human oversight and AI autonomy depends on the application

The **scope of model responsibility** is an important, and complex, issue. If AI systems disclose potential harm from their suggestions, the responsibility lies with the human user who ultimately enacts those suggestions. However, as AI systems gain autonomy and make decisions without human intervention, this responsibility becomes less clear. Striking the right balance between human oversight and AI autonomy is vital for responsible AI deployment. The need for this will vary depending on the application. It is, for example, less of an issue in using AI/ML for experimental design, where the consequences of a problem with the model are simply more failed experiments, and the experiments themselves validate or disprove the ML predictions. It will be much more of an issue as AI/ML is more widely used for automated decision making in downstream production processes. Here, the factors driving how models respond to new inputs need to be much more clearly understood.

Addressing **bias** in AI systems is also critical for responsible deployment and fostering trust. AI developers must proactively identify and mitigate bias during model development. Regular audits and bias assessments can help ensure AI systems are fair and inclusive. Incorporating human oversight in AI decision-making will help to detect and correct biased outputs, reinforcing responsible use. Research by [15] agrees that the relationship between human and AI should be intertwined, with benefits of either being exploited and shortcomings omitted.

Feasibility study results

Key conclusions

A step change in the application of ML is inevitable – how can we accelerate its benefits?

We found strong support for the idea that a step-change in the application of machine learning to support innovation in the industries studied is both desirable and achievable. Indeed, given the rapid continued development of computational technologies, such a transition is inevitable. Competitive benefits will accrue to companies, industry sub-sectors, and geographical regions where this change occurs most rapidly. The change will primarily be driven by individual research organisations making smart ROI decisions in a competitive commercial market for AI/ML technology vendors, informed by growing evidence of the value of the technology. But this process can be accelerated and facilitated by proactive steps to mitigate organisational and cultural barriers to adoption, by industry-level education initiatives, and by vendors optimising their offerings. We identified potential action areas.

Educational and organisational issues

Our study identifies scope for action in three key areas relating to the human and organisational aspects of AI/ML adoption in the industry:

1. **Encouraging effective sponsorship and leadership** within chemicals and materials companies. AI/ML adoption should be built into strategic objectives. Teams should be empowered with the time and resources needed to implement and optimise AI/ML in real workflows. Inertia can be addressed by providing support, training, and encouragement from leadership, fostering a culture that embraces change and innovation, while setting clear milestones for multiphase projects. This protects organisational interests while building trust in implementations as milestones are met.

2. **Educational initiatives at the industry level** could promote better understanding of AI/ML technologies, particularly among the wider audience of chemists and materials scientists who are potential users. This education should include an introduction to AI/ML ('what is an ML model?'), explanations of potential applications, discussion of potential limitations and challenges in applications, and what to look for in an effective AI/ML project. Participants felt that such education would be most effective if delivered as practical, hands-on training, ideally based on exercises that could be applied to real projects within the workplace.

> Initiatives are needed at organisational and industry levels to build trust in AI/ML

3. **Alignment with key industry strategic objectives** – there was agreement that clearer understanding of how AI/ML can assist with key industry objectives would help to drive sponsorship and implementation of projects. Alignment with **net zero** objectives should be emphasised, given the scope for the technology to assist in the multi-parameter optimisation problems associated with improving the environmental performance of formulations, chemicals, materials, and processes.

Technology and tools

The project also identified some key requirements for AI/ML tools for the chemicals and materials industries. This checklist that can be used both by vendors of such technology and by anyone considering implementing such technology in their organisation:

> Anyone implementing AI/ML projects can use this checklist

1. **Explainable AI** – solutions must provide tools to increase the explainability and transparency of ML models and resulting decisions.

2. **Bias and uncertainty** – solutions must provide straightforward ways for users to establish confidence in their results, understanding their biases and the uncertainty in their predictions.

3. **Task-centric user interfaces** – solutions should pay close attention to making AI/ML technology easy to access and use within the workflow of chemists and materials scientists, through UI design based around the tasks that these scientists need to accomplish (e.g., experimental design) or integration within existing tools.

4. **Handling real experimental and process data** – ML methods will be easiest to implement when they work 'out of the box' with the sparse, noisy data typical of experimental and process datasets. Depending on the application, they may need to either produce useful insights from small datasets, or handle the computational challenges of large datasets, or both.

5. **Matching the solution to the application** – for example, more tools to establish trust and monitor biases and uncertainty are required in applications where the AI is given more autonomy than in those where it is, for example, recommending experiments the results of which will validate its predictions.

6. **System and data integration** – solution providers and in-house IT teams must think carefully about how AI/ML tools interact with other tools and with the flows of data within the teams applying them. The goal should be to minimise the friction caused by introducing new tools into existing processes and to ensure that they add value.

Conclusion

This project has explored some of the issues around adoption of AI technologies, particularly ML, in the chemicals and materials industries. We have found strong industry interest in adopting these technologies, particularly, initially, in R&D. And many organisations have made a good start, often with positive outcomes. Those that are yet to implement AI/ML at all in areas such as design of experiments are certainly behind the curve. But we have also found plenty of scope to widen, deepen, and accelerate this implementation in every organisation studied, with current projects often confined to expert project teams or a small number of pilot projects.

We identified some of the key issues that might act as a brake on the adoption of this technology and suggested some areas on which to focus future efforts – both for industry-wide educational activities and organisational principles, and for vendors and users of relevant software technology. More detailed analysis and action in each of these areas might be the focus for future industry collaboration.

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About Intellegens

Our mission is to be the leading machine learning solution for real-world, sparse and noisy data problems in industrial R&D and manufacturing processes. Our focus is on making it easy to apply machine learning to accelerate innovation. Alchemite™ originated at the University of Cambridge and development is on-going at Intellegens, in close collaboration with our growing community of Alchemite™ customer organisations. These represent sectors including alloys, additive manufacturing, aerospace, batteries, ceramics, chemical processes, composites, consumer products, cosmetics, drug discovery and development, energy, food and beverage, formulated products, paints, plastics, printing technology, and translational medicine.

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