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The Role of AI across Battery R&D and Manufacturing



AI generated image

Mona Faraji Niri, Associate Professor, WMG, University of Warwick
John-Joseph Marie, Principal Analyst, Faraday Institution

Artificial intelligence is accelerating the pace of scientific discovery. Its impact on battery innovation could be far-reaching, advancing materials discovery, cell design and manufacturing, while shortening development timelines and improving battery performance. For the UK, the opportunity is substantial, but so are the consequences of falling behind in a technology set to define the next era of industrial competitiveness. Realising these benefits will require closer integration of data and AI tools across the battery value chain, supported by high-quality data, trusted models and interdisciplinary collaboration.

Introduction

Artificial intelligence (AI) is opening unprecedented possibilities for scientific discovery, with breakthroughs previously thought to be decades away now being achieved in a fraction of the time. A notable example is Google DeepMind's AlphaFold, which has accelerated the prediction of protein structures from years to minutes, a breakthrough recognised with the 2024 Nobel Prize in Chemistry.[1] AlphaFold has since predicted the structure of over 200 million proteins and is used by over three million researchers globally, saving an estimated hundreds of millions of research years.

Policy initiatives are being developed to match the scale of the opportunity. The Genesis Mission, launched in November 2025, is a US programme building a national AI-for-science ecosystem, aiming to double the productivity of American science within a decade through AI.[2] However, AI's potential is not confined to research: it is increasingly seen as a general-purpose tool capable of transforming innovation, manufacturing and operations across industry. This is reflected in considerable investment in AI-related infrastructure, with over $1 trillion being invested from big tech hyperscalers (Google, Amazon, Meta, and Microsoft) since 2023.[3] Another example is the AI Materials Foundry led by UK based CuspAI, which brings together 45 organisations forming a global network of data, labs, compute and scientific expertise to accelerate materials discovery.[4] The opportunity for the UK is substantial, with AI set to define the future of scientific discovery and industrial competitiveness.

This Insight considers what this opportunity means for the battery sector. Batteries are becoming increasingly critical, with rising demand and highly concentrated global supply chains highlighting the need for innovative approaches to battery R&D and manufacturing.[5] The inclusion of both batteries and AI within the UK's Modern Industrial Strategy highlights the importance of developing UK capabilities in both technologies to support future economic growth and industrial resilience.[6] Strong domestic AI expertise could support the UK's competitiveness by accelerating innovation in established and next-generation battery chemistries.

In battery R&D, AI can complement traditional modelling and experimentation by identifying relationships between battery materials, cell designs, operating conditions and performance

[1] Google DeepMind - Alphafold.
[2] U.S. Department of Energy - Genesis Mission.
[3] Financial Times - Big Tech AI spending spree tops $1tn (July 2026).
[4] Business wire - CuspAI Launches 'AI Materials Foundry' to Accelerate Breakthrough Discoveries (July 2026).
[5] IEA - Global battery markets are growing strongly – and so are the supply risks (February 2026).
[6] UK Government – The UK's Modern Industrial Strategy (November 2025).

UK Government
UKRI Innovate UK

to design better batteries. Automated labs are also demonstrating how development cycles for current and next-generation battery chemistries can be accelerated. However, AI should not be viewed as a single technology, but rather as an extensive set of tools and techniques that can be applied to different challenges across the value chain.

While AI-enabled tools are already being deployed across the battery industry, their wider adoption faces several challenges. These include the limited availability of datasets of sufficient quality and consistency for training reliable models and the need for interdisciplinary expertise spanning battery science, engineering and data analytics to develop, validate and interpret AI outputs.

This Insight provides an overview of AI and how it is being deployed across the industry. It then presents case studies of existing AI deployments across the battery value chain and discusses the future role of AI in battery innovation. Finally, it outlines the critical challenges facing broader AI adoption across battery research.

An Introduction to Artificial Intelligence

Overview of AI

AI refers to computer systems using data-driven methods to support problem solving and decision making in ways that mimic human intelligence. The term 'artificial intelligence' was coined in 1955, amid the development of early neural networks and machine learning (ML) approaches.[7]

ML is a subfield of AI focused on systems that learn patterns from data, drawing on several fields including statistics, linear algebra and optimisation theory.[8] ML algorithms underpin AI tools in use today and are commonly grouped into three main classes, namely supervised learning, unsupervised learning and reinforcement learning. These differ in how much labelled data and human guidance they require.[9] AI can be categorised into the following three broad groups:

- **Narrow AI** refers to AI that can be trained to perform a single task, far faster and better than humans, but that cannot perform beyond its defined task.
- **General AI** can use previous learning and skills to perform new tasks in a different context without requiring further human intervention needed to train the underlying models.
- **Super AI** is expected to think, reason and make decisions and judgments better than humans.

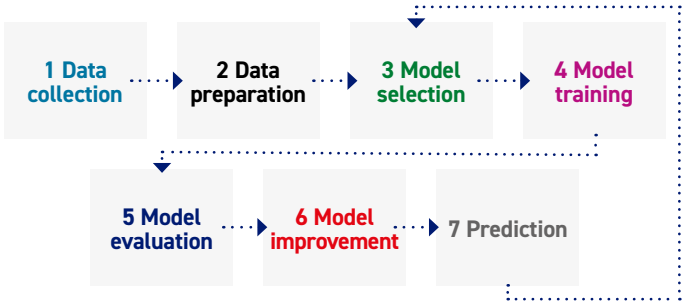
Within Narrow AI, models are commonly grouped by what they are trained to do. Predictive AI models learn from historical data to forecast an outcome or classify an input and are typically built using classical ML methods.[10] Generative AI models instead learn the underlying patterns in data well enough to produce new, original outputs rather than predicting a value.[11] Increasingly, both are being developed from foundation models: large models pre-trained on broad datasets, which can be adapted or fine-tuned for specific tasks rather than built from scratch.[12]

While General and Super AI remain theoretical concepts, Narrow AI forms the basis for the AI tools of today. As a stepping stone towards General AI, many AI companies are pursuing Agentic AI, which can coordinate multiple AI capabilities and external tools or resources to apply knowledge across different tasks, achieving broader goals than task-specific Narrow AI systems.

AI model development

The development of an AI model involves training a computational model using data relevant to the task of interest. AI and ML models learn statistical relationships within the data (Figure 1), allowing them to perform tasks such as regression, classification, or content generation. Once trained, the model can be applied to new data enabling the rapid and consistent execution of the specified task.

Figure 1: The seven stages of AI model development – a simple workflow



Recent improvements in AI tools have led to an increasing uptake of AI across industry (Box 1). These advances have come from taking advantage of growing volumes of training data and rapid advances in computational hardware, allowing AI systems to be scaled up in three key ways:[13]

- **Increased model size**: The size of an AI model can be characterised by the number of parameters the model has that are adjusted during training to improve performance. Increasing the number of parameters expands the range of patterns and relationships the model can represent, enabling the model to learn more effectively from large datasets.
- **Increased data availability**: AI systems are trained on datasets to identify and learn from patterns in the data. Using larger volumes of data to train these models improves performance by capturing the nuances and complexities of real-world patterns and behaviours. Although dataset size is important, the quality, diversity and representativeness of data also play a critical role in determining how well AI models perform and how reliably they adapt to new situations.

[7] IBM - The history of artificial intelligence.
[8] IBM - AI vs machine learning vs deep learning vs neural networks: What's the difference?
[9] IBM - Five machine learning types to know.
[10] IBM - What is predictive AI?
[11] IBM - What is generative AI?
[12] IBM - What are foundation models?
[13] Our World in Data - Scaling up AI (January 2025).

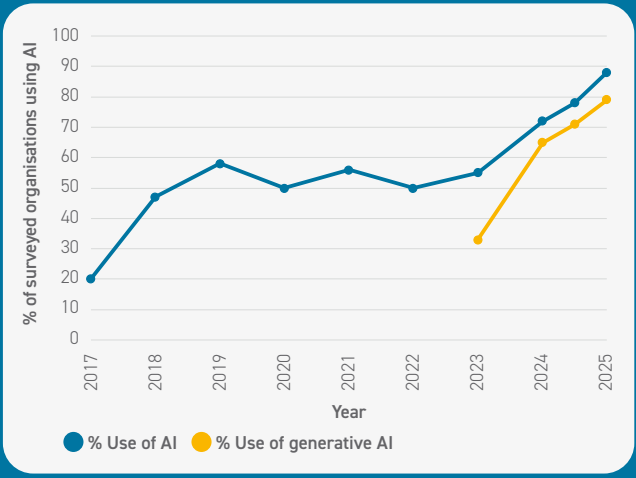
Box 1: The uptake of AI in industry

The use of AI has increased dramatically throughout the economy. A recent McKinsey survey of around 2,000 respondents found 88% of organisations reporting the use of AI in at least one business function, up from 55% in 2023 (Figure 2).[14] Adoption was similarly widespread in advanced manufacturing, where 86% of organisations surveyed reported using AI in at least one business function. However, only 7% of organisations using AI had fully integrated it, while a further 31% were scaling the use of AI across their organisation. This suggests that, although AI is now widespread, deep integration remains the exception rather than the norm.

AI is also being used to accelerate innovation, with 64% of respondents reporting that AI has enabled innovation at their organisation,[14] while R&D and innovation have been identified as one of the largest sources of potential value from AI.[15] Applying AI directly to scientific and engineering workflows can deliver substantial improvements. In the chemicals sector, closed-loop research systems train AI models on laboratory or simulation results and use them to guide the next round of experiments. In some cases, these systems have reduced the number of R&D iterations and the amount of data required by 90-99% compared with conventional AI approaches and could more broadly double the overall pace of R&D.[16]

Although AI adoption is growing, the financial benefits vary widely. Only 39% of organisations report any impact on company-wide operating profit, with most estimating that AI is responsible for less than 5% of profit. That said, many organisations have seen cost savings or revenue gains from specific uses of AI, including product development and manufacturing.[14] Only a small group of high-performing companies report that AI is responsible for 5% or more of their operating profits. These companies tend to use AI not only to reduce costs but also to support innovation and growth, with AI typically being integrated into workflows. Another survey suggests that financial benefits are also concentrated among a small number of companies, with 5% of companies surveyed achieving about five times the revenue gains and three times the cost reductions of less advanced companies.[15]

Figure 2: Use of AI across organisations



Source: McKinsey Global Surveys on the state of AI, 2017-2025.

- **Increased compute**: Training larger models on larger datasets has been made possible through significant improvements in computational hardware. Advances in specialised processors, including GPUs and TPUs,[17] have been optimised for large-scale parallel operations, dramatically increasing throughput compared with traditional CPUs.

How will AI impact battery R&D

AI in scientific and industrial settings (including battery applications) can be grouped according to how AI is deployed to support R&D tasks, each with different maturity levels:[18]

- Applying predictive AI models to optimise manufacturing processes or predict the properties of established materials from data. These applications are mature and increasingly employed in battery manufacturing and R&D activities today.
- Developing AI systems that assist scientists with research tasks, such as helping researchers navigate large materials design spaces or interpret complex experimental datasets. These applications are emerging, drawing on large language models (LLMs) and Agentic AI tools to coordinate activities.[19]
- Developing autonomous AI systems capable of generating and testing new hypotheses with limited human guidance, such as closed-loop systems that propose experiments, run them via automated or robotic platforms, and interpret the results to inform the next iteration. These applications are still at an early stage of development.

Together, these capabilities point to a new approach to R&D. Rather than treating data collection, modelling and experimentation as separate, sequential steps, AI could eventually weave them together into a single, iterative process. This will rely on a broad array of complementary AI tools each suited to different tasks and at different stages of maturity. To ensure AI succeeds in battery-related applications, organisations in academia and industry must approach AI adoption as a transformational change in R&D and manufacturing, rather than as an incremental initiative.

[14] McKinsey - The state of AI in 2025: Agents, innovation, and transformation (November 2025).
[15] BCG - The Widening AI Value Gap (September 2025).
[16] McKinsey - How AI enables new possibilities in chemicals (November 2024).
[17] IBM - What is AI hardware? CPU, GPU, TPU and other definitions in the glossary.
[18] Stanford University Human-Centred Artificial Intelligence - AI Index Report 2026.
[19] W. Zhuo et. Al., Large language models for batteries, Joule, 2025.

AI should not be viewed as a single technology, but rather as a collection of different tools and approaches designed for specific tasks. Different AI tools rely on different datasets, assumptions and objectives, meaning tools developed for materials discovery may not be suitable for manufacturing optimisation or diagnostics.

Current State-of-the-art Applied AI in Battery Research and Industry

As global AI adoption accelerates, its applications are expanding across the battery value chain, from research and development to manufacturing. This section demonstrates the breadth of AI's current application, from materials discovery through to manufacturing and in-service diagnostics. The examples presented in this section are illustrative rather than exhaustive, with further applications foreseeable across the battery value chain.

Material discovery

The battery anode, cathode and electrolyte are critical components of batteries that determine battery performance. However, their development using traditional research methods can be slow and heavily iterative. AI-based approaches address this in two ways. Predictive AI models can screen large numbers of candidate materials against constraints such as cost, composition and physical properties, rapidly narrowing a design space that would be impractical to explore manually. More advanced generative tools support target-based materials design, in which researchers specify desired properties and the AI proposes novel candidate materials to meet the requirements, reversing the traditional discovery process. These approaches can accelerate the identification and evaluation of novel materials and the subsequent development of new battery chemistries (Box 2).

Battery electrode, cell and pack design

The choice of active materials largely determines the behaviour of the cell. However, the same cell chemistry can deliver very different performance levels depending on cell parameters such as electrode thickness or cell form factor (e.g., cylindrical, prismatic). A key component of this is the electrode microstructure, the properties of which affect the performance of the cell and can be optimised during electrode manufacturing. However, this requires iterative testing costing time and material resources. Generative AI approaches are being used to accelerate this process by simulating electrode microstructures with pre-determined performance targets (Box 3). The Faraday Institution's Nextrode project is also looking to build on these approaches as part of its mission to advance next-generation electrode manufacturing.[24]

Cell and pack design also involves numerous interdependent factors, including cell format, thermal management, lifetime, manufacturability and cost. The complexity of these design spaces makes exhaustive testing and manual optimisation impractical. AI-based modelling approaches are already being used to accelerate cell and pack design. LG Energy Solution, for example, has developed models

Box 2: AI for materials discovery

Materials discovery is increasingly supported by advanced AI tools that both generate new candidate materials and rapidly evaluate their properties to accelerate screening and selection. Materials discovery platforms are emerging which have the potential to accelerate the pace of materials discovery. UK-based CuspAI is a deep-tech startup that operates as an AI-powered search engine for material design to accelerate material discovery. The company has recently raised $450 million from investors including the UK Government, alongside announcements of the launch of AI Materials Foundry, a global network of 45 organisations including NVIDIA, Meta, and the Henry Royce Institute.[20] The initiative brings together the infrastructure required to enable researchers to develop new materials, targeting discoveries in semiconductors, clean energy and advanced manufacturing.

Another example is Orbital Industries, a London- and San Francisco-based startup using AI to simulate atomic-scale material behaviour to accelerate materials discovery. Orbital is vertically integrated plans to sell the materials its models discover directly. The company has signalled ambitions to extend this model beyond data centre applications into broader materials discovery.[21]

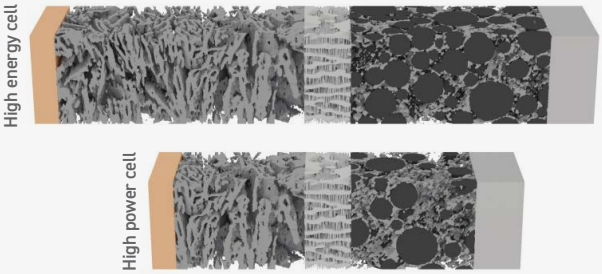
Beyond general material discovery platforms, there are also examples from the battery industry. CATL has used AI models to pre-screen large numbers of candidate materials in search of ideal chemical systems, reducing the time required for materials screening to around one-hundredth of that required by conventional methods. In solid-state battery development, this approach enabled CATL's R&D team to identify seven target materials in three months while improving ionic conductivity.[22] A second example is Intellegens which has designed an algorithm to train on the sparse, incomplete datasets typical of materials research, collaborating with Ansys UK and the University of Birmingham on battery-related work.[23]

[20] Reuters - UK government, Bezos back CuspAI's $450 million round as startup seeks to discover new materials (July 2026).
[21] Fortune - Orbital Industries, startup using AI to discover exotic new materials, raises $50 million Series B funding round (May 2026).
[22] CNEV Post - CATL chief scientist explains how AI accelerates battery R&D (May 2026).
[23] Intellegens - Formulation and manufacturing of batteries (December 2021).
[24] Nextrode.

Box 3: AI tools for battery electrode, cell, and pack design

Researchers at Imperial College London have demonstrated how AI can accelerate battery electrode design. Using a small number of electrode images, the AI tool generates 3D electrode microstructures across a range of design parameters, reducing the need for trial-and-error testing. Figure 3 shows examples of electrode structures optimised for power and energy applications. This research led to the creation of Polaron, a spin-out company from Imperial College London that uses AI-based modelling approaches to accelerate microstructure development. Polaron's models can explore thousands of candidate microstructures in under a day, a task estimated to take 50 years using existing physics-based simulations. These models have also demonstrated improvements in battery energy density of more than 10%.[25]

Figure 3: Synthetic microstructures for energy and power cells by generative AI models



Source: S. Kench et al., Li-ion battery design through microstructural optimization using generative AI, Matter, 2024. In both images, from left to right, the figure shows a copper current collector, a graphite electrode, the separator, an NMC cathode, and an aluminium current collector.

that automatically generate and verify battery cell designs based on customer requirements. These models, which use data from 100,000 cell designs and generative AI techniques, reduce the time required for cell design from two weeks to one day.[26] Another example is UK-based IONETIC, which has developed Arc, a suite of AI design tools that automate battery pack design. The company reports that this approach roughly halves the time to market and reduces development costs.[27]

Cell manufacturing

Efficient and reproducible cell manufacturing at scale is required to ensure that cells can be made safely, consistently and cost-effectively. Cell manufacturing is a highly complex and tightly controlled multi-step process, where small variations in parameters can significantly affect cell performance and process yield. ML-based approaches are expected to play a pivotal role in optimising future cell production and supporting a competitive battery manufacturing industry.[28] These methods identify hidden correlations between manufacturing conditions and cell quality to optimise process parameters in real time, improving manufacturing efficiency and cell quality control (Box 4).

A key bottleneck in lithium-ion battery manufacturing is formation and ageing, a process that can take several weeks and ties up significant capital and factory floor space before cells are ready for shipment. The Faraday Institution's FAST project, led by the University of Birmingham, is applying AI-driven diagnostics, hybrid physics-based modelling and ML to accelerate this step.[29]

Box 4: Applications of AI across cell manufacturing

AI and ML based approaches are being used across cell manufacturing to improve process efficiencies and quality control. Voltaiq, a US-based start-up, provides a battery intelligence platform that produces insights into cell performance and quality.[30] It applies ML to data collected from manufacturing processes to identify trends and detect anomalies more quickly than traditional quality control methods, tracing issues back to specific materials or process steps. AI-enabled image analysis is increasingly being combined with X-ray computed tomography scanning to support quality control of lithium-ion cells by identifying internal manufacturing defects that can affect performance and safety.[31] Some ML approaches are now sufficiently mature for industrial use and have been deployed by a number of battery manufacturers such as EVE Energy in smart manufacturing approaches.[32]

Digital twins (virtual models that use AI-based approaches to predict how changes in production affect cell quality, reducing the time and cost of physical trials) are also being explored, although such initiatives remain at the pilot stage. An example is the Horizon EU-funded BATTWin project involving WMG, that is developing a multi-level digital twin platform to reduce defect rates in battery production.[33]

[25] Henry Royce Institute - AI that rapidly designs advanced materials for batteries wins first Manchester Prize (March 2025).
[26] Battery Technology - LG Energy Solution Unveils AI-Powered Model to Slash Battery Cell Design Time (July 2024).
[27] IONETIC slashes EV battery pack development time and costs, unlocking multi-million-dollar savings (October 2024).
[28] Fraunhofer - Mastering Ramp-up of Battery Production (October 2024).
[29] The Faraday Institution - FAST - Formation and Aging for Sustainable Battery Technologies.
[30] Voltaiq.
[31] Bestmag - Lumafield reports on lithium-ion 18650 cell quality (September 2025).
[32] EVE Energy - EVE Energy Sets a New Benchmark in Smart Manufacturing (January 2026).
[33] BATTWin.

Across applications from materials discovery to manufacturing and diagnostics, AI-based tools are enabling researchers and engineers to explore larger design spaces, identify issues earlier and reach results with fewer physical experiments or iterations than conventional approaches alone, delivering time and cost savings.

Battery diagnostics and battery management systems

Monitoring and controlling battery performance in real time to ensure safety and longevity are the roles of battery diagnostics and the battery management system (BMS). Diagnostics refers to the estimation of several key internal states, including state-of-charge, internal resistance and temperature, using data collected from sensors within the pack. The resulting data is then fed into the BMS, which acts as the control layer of the battery pack, managing cycling rates, cell balancing and thermal conditions within the pack to prevent thermal runaway.

AI models can enhance battery diagnostics and BMS operation by estimating internal cell characteristics such as state-of-health and remaining useful life more accurately, or by detecting early signs of degradation from patterns in sensor data. These approaches are complementary rather than competing with established methods: because purely data-driven models can behave unpredictably outside their training conditions, integrating AI with physics-based electrochemical and thermal models (techniques that have long underpinned battery research)[34] improves reliability by keeping predictions physically consistent, combining data-driven flexibility with established scientific understanding. Box 5 presents examples of these innovations being developed in industry.

Beyond these diagnostic and BMS capabilities, physical AI is an emerging approach that embeds sensing, reasoning and, eventually, actuation directly within the cell itself, rather than relying on sensors and control logic positioned around it. The Horizon Europe-funded SALAMANDER project, for example, integrates sensors directly into cell electrodes and uses a physics-based model to interpret degradation signals at the source to detect degradation and trigger a protective or self-healing response autonomously, without relying on an external BMS.[35] The technology remains at an early stage but illustrates how far diagnostics and BMS technology could extend.

Automated laboratories

Automated laboratories shift research from manual, trial-and-error experimentation towards fully integrated, data-driven research environments. By combining high-throughput experimentation, robotics and AI, automated labs can design, execute and analyse experiments with minimal human intervention. This helps improve reproducibility while generating large, structured datasets for model development. This is particularly valuable in battery research, where vast materials design spaces and complex processes make conventional experimentation inefficient. AI-enabled laboratories with robotics are beginning to be deployed across academia and industry (Box 6).

However, this capability comes with significant upfront costs. Automated laboratories require substantial planning to define the experimental space, design protocols and robotics workflows, and validate the outputs from automated experiments. In addition, human input is often still required to define experimental objectives, configure workflows, interpret unexpected results and intervene when experiments or equipment fail.[39] Once built, these systems also tend to be inflexible, as they are optimised for a specific class of materials or workflow. Adopting these systems therefore needs a long-term commitment to a particular application.

Box 5: AI tools for battery diagnostics and battery management systems

AI tools are increasingly used in battery diagnostics to improve performance monitoring, lifetime prediction, safety and operational control under real-world conditions. UK-based Generational uses data-driven analytics to assess EV battery condition, including battery health checks and state-of-health estimation to inform second-life and end-of-life decisions. The 2025 Battery Performance Index, based on tests of over 8,000 EVs in the UK, found an average state-of-health of around 95%.[36]

AI tools are also being used across BMS development. Elysia, part of Fortescue, combines physics-based models with ML to improve performance, safety monitoring and energy management, particularly in high-demand applications such as off-road and motorsport vehicles, and has demonstrated up to a 30% increase in battery life.[37] UK-based Eatron also integrates AI into BMS to maximise battery performance through predictive diagnostics that identify early signs of degradation or failure and extend battery life by up to 25%.[38]

The Future Role of AI in Battery Innovation

An overview of AI-led experimentation

The benefits of AI and ML approaches are already being seen across industry. However, current applications still generally operate within a defined stage of the battery value chain, whether in R&D, advanced manufacturing or system diagnostics, with humans connecting these stages together. The most ambitious but least mature form of AI deployment is AI-led experimentation, where autonomous systems

[34] Faraday Insight 15 - The Value of Modelling for Battery Development and Use (December 2022).
[35] SALAMANDER Project.
[36] Batteries News - UK's largest used-EV battery study reveals 95% average battery health (February 2026).
[37] Snowflake - Elysia Boosts Battery Life by 30% for a More Energized World.
[38] Eatron - A Revolutionary Battery Management Solution: AI-BMS on Chip (June 2024).
[39] H. Lee et. al., Toward self-driving laboratory 2.0 for chemistry and materials discovery, Mater. Horiz. 2026.

Box 6: Automated approaches to R&D in academia and industry

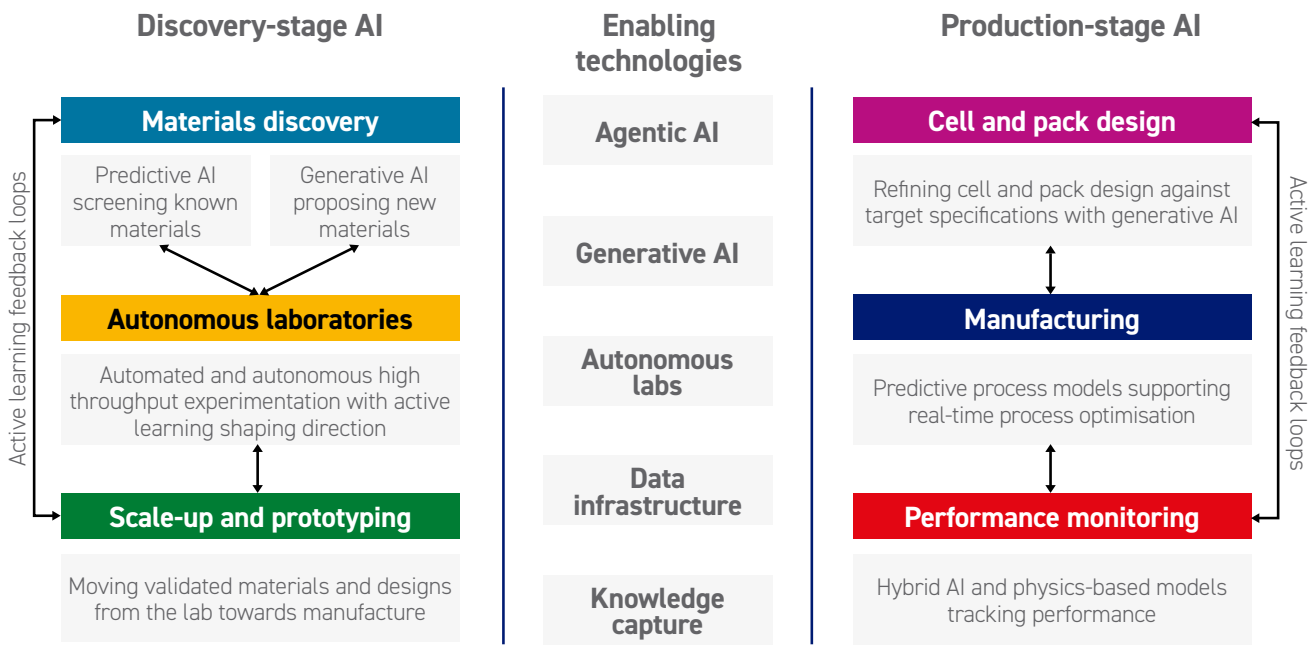
In 2023 Imperial College London launched DIGIBAT, a self-driving laboratory designed to accelerate energy materials discovery.[40] DIGIBAT integrates AI with robotics across the full experimental pipeline, from materials synthesis and electrode fabrication to coin cell assembly and electrochemical testing. This bridges the gap between atomic-scale design and cell-level validation. Its high-throughput, standardised workflows enable hundreds of experiments to be conducted with high reproducibility, reducing discovery timelines from years to months while producing high-quality datasets. In July 2026, the DIGIBAT team released the Discovery Benchmark, an open dataset of around 250 lithium-ion coin cells built on the facility's automated assembly platforms, with characterisation and electrochemical data linked to individual cell records and annotated using the BattINFO ontology. Supported by the Henry Royce Institute, DSIT and UKRI, it demonstrates the full digital thread from robotic equipment through structured databases into AI systems.[41] Similar approaches are being deployed by research groups around the world, demonstrating a shift in how materials discovery is being approached in academia.[42]

These approaches are also being deployed across industry. LG Energy Solution recently discussed their approach to AI integration across innovation and manufacturing through their 'Virtual Lab' and 'Dark Factory' initiatives. Virtual Lab spans materials screening, generative cell design tools and AI-based visual inspection of results, while Dark Factory applies AI to detect defects, optimise manufacturing processes and automatically adjust the production line itself. These efforts allow data collected during manufacturing to be fed back into the design models used in R&D, while designs generated virtually are implemented directly on the production line, creating a continuous exchange between design and manufacturing.[43] Another example comes from CATL, whose long-term vision is to develop large model-driven, high-throughput autonomous laboratories capable of accelerating battery innovation through AI-guided design, automated experimentation and autonomous validation workflows.[22]

generate hypotheses, design and run experiments, interpret results, and decide where to focus next in a closed loop. This shifts human oversight from execution towards strategic direction and validation.

Figure 4 outlines how an AI-led experimentation system could operate through a discovery-stage loop centred on materials discovery and autonomous laboratories, connected to a production-stage loop centred on cell design, manufacturing and performance monitoring.

Figure 4: A depiction of an AI-led battery R&D system, from discovery to production



[40] Imperial - DIGIBAT.
[41] Henry Royce Institute - Discovery Benchmark Released: Open Battery Dataset Showcases the Future of AI-Enabled Materials Discovery (July 2026).
[42] UC Berkeley, Ceder Group - Autonomous experimentation for accelerated materials discovery.
[43] Battery Inside - How Is AI Used in the Battery Industry? AI Applications Across LG Energy Solution's R&D and Manufacturing Operations (June 2026).

The benefits of such a system include shorter R&D timelines for new battery chemistries, increased efficiency of production and improved performance from cells and packs. Elements of this vision are beginning to emerge across R&D in academia and industry (Box 6). However, delivering such a system will require buy-in from stakeholders and further development of enabling technologies.

Enabling AI-led experimentation

Several key infrastructure components must be developed to support AI-led experimentation. The first requirement is the development of the physical infrastructure to enable autonomous and high-throughput experimentation. Automated laboratories such as DIGIBAT illustrate how robotics combined with AI can enable high-throughput experimentation but are typically purpose-built for specific workflows, limiting their flexibility and wider deployment. Developing more modular and cost-effective automation platforms will therefore be essential to enable broader adoption.[39]

The second is the development of the required digital infrastructure that can reliably predict novel materials based on a target set of properties. Diffusion models have emerged as one of the leading approaches for generative materials design, with several examples demonstrating progress towards creating foundational generative models for materials design.[44,45] The role of academic-led research is crucial: the Stanford AI Index identifies that most AI models for science originate from academic and government institutions, in contrast to the industry-dominated general-purpose AI landscape.[18]

In addition, software capable of orchestrating increasingly complex workflows will be necessary. Today, researchers often still translate AI-generated proposals into executable protocols manually. LLMs are emerging as a promising way to coordinate this process.[19] Looking further ahead, this role could extend to Agentic AI systems coordinating materials design, experiment planning, laboratory control and data analysis with minimal human intervention.[39] However, achieving this level of coordination will depend on improvements in interoperability and standardised software interfaces.

A third requirement is the infrastructure needed to capture, store and reuse data generated across the value chain. AI-led experimentation will require the consistent collection of data from each stage, whether from a synthesis run, a manufacturing line or a cell in operation, and its incorporation into subsequent iterations. Data management is a persistent challenge in battery R&D, where data is often fragmented, inconsistently recorded, or lost between systems and stages. Without appropriate data infrastructure, insights generated at one stage remain isolated rather than informing other stages of the research process.

A further often overlooked gap concerns how existing human expertise is captured and used. Much of the knowledge that determines success is qualitative and experience-based, held by engineers rather than recorded in structured datasets. Ontologies and knowledge graphs formally encode expert-defined relationships between materials, processes, and performance outcomes, embedding experience-based knowledge into AI systems in a machine-readable form. Initiatives such as BattINFO, a battery-specific ontology standardising terminology across the sector, represents early steps in this direction.[46] This is beginning to be applied to real data, as the Discovery Benchmark dataset highlighted in Box 6 illustrates.

The scale of investment this vision requires is substantial, but examples are already underway. The US Genesis Mission illustrates what a deliberate attempt to build this infrastructure looks like in practice. Alongside its goal of doubling US scientific productivity, the programme has secured over $5 billion in Federal commitments across 15 agencies to invest in shared compute, standardised data infrastructure, and AI-driven experimental platforms.[47] UK-

Box 7: Towards a UK 'Faraday Engine'

The UK is developing systems that use AI to plan, run and adapt battery experiments, centred on the national research facilities at Harwell. Dr James Le Houx (University of Greenwich; STFC/Faraday Institution Emerging Leader Fellow, hosted at ISIS Neutron and Muon Source) works on autonomous decision-making for battery characterisation at large-scale facilities, and has built engagement across the battery community in neutron, muon and X-ray techniques through a series of Faraday Masterclasses.

Building on this, a collaboration between STFC's national facilities and the Faraday Institution brought together facility directors and technology leads with research leaders from across the Faraday Institution's core projects. The collaboration set out a vision for a "Faraday Engine": an AI-powered platform coupling automated synthesis with autonomous characterisation at national beamlines. National facilities offer multimodal, high-resolution and fast measurements that laboratory instruments cannot match, whether applied to screening large sample libraries or to probing a sealed cell in operation without taking it apart. Delivering this would place the UK among the leaders in AI-led battery research.

Work towards this has already started. A recent collaboration at Diamond Light Source demonstrated automated robotic sample handling for battery research, screening up to 150 samples per day within a single experiment. The next step is closing the loop, feeding analysis back into experimental decisions while measurements are being taken.

[44] H. Park et. al., Exploration of crystal chemical space using text-guided generative artificial intelligence, Nature Communications, 2025.
[45] C. Zeni et. al., A generative model for inorganic materials design, Nature, 2025.
[46] BIG-MAP - BattINFO Project.
[47] The White House - More Than $5 Billion for the Genesis Mission, a National Mission on AI for Science (July 2026).

based initiatives include efforts from the Faraday Institution, the Hartree Centre and US national laboratories, who convened a joint UK-US workshop on exascale computing and AI in November 2025, leading to a workplan to co-develop shared research capability and facilities.[48] The UK is also pursuing a vision for AI-led experimentation centred on a proposed 'Faraday Engine' at the national research facilities in Harwell (Box 7). Increased investment and longer-term collaboration will be critical to ensure that infrastructure access does not become a bottleneck to productivity, scale-up and innovation.

The evolving role of human expertise

Even as AI-led capabilities mature, human expertise will remain indispensable, though its role will shift. AI can accelerate exploration and support decision-making. However, assessing if novel material candidates justify the cost of physical validation (a key bottleneck), or setting the direction of a research programme will continue to depend on scientific judgement that current AI systems cannot replicate. The likely near-term outcome is thus not the replacement of researchers but a change in how they apply their expertise towards designing, overseeing and validating increasingly autonomous systems. Establishing such systems will ultimately depend on collaboration between battery researchers and AI specialists, rather than either group working in isolation.[19]

Challenges Facing AI Adoption

While AI is rapidly advancing, it is important to remain realistic about near-term capabilities with respect to battery development. Realising AI's potential in battery R&D therefore depends on addressing a set of interconnected challenges, spanning the availability of high-quality data, the skills needed to develop and apply AI effectively, trust in model outputs, and the ability to validate AI-generated insights against physical reality. Beyond these technical barriers, wider adoption also depends on access to the powerful computational infrastructure that AI requires and on developing organisational cultures that supports the integration of AI into existing ways of working (Figure 5).

Figure 5: Barriers to the adoption of AI in battery R&D



Data

Data is a key enabler for AI-based approaches. Progress in developing AI tools is often constrained by the availability of high-quality, application-specific data, which is increasingly being viewed as essential research infrastructure for AI tools in battery R&D. Poor or biased datasets can embed systematic errors that are hard to identify, making it difficult to develop models that generalise reliably beyond the conditions represented in that data. For example, a model trained on coin cell data may not reliably predict performance in commercially relevant cell formats. In practice, battery datasets are often fragmented and collected under differing protocols with limited shared metadata. Figure 6 outlines the requirements for a robust, representative and high-quality dataset.

Figure 6: Factors contributing to ensuring the quality of an AI dataset



To address these challenges, there are several coordinated initiatives across industry and academia to develop open battery data standards and frameworks. One example is the Battery Data Format (BDF) initiative led by the LF Energy Battery Data Alliance, which aims to define a common, machine-readable structure for experimental and simulation battery datasets.[49] This format will improve collaboration between academia and industry to develop AI tools by improving consistency, reproducibility and compatibility between data sources. BDF builds on contributions from across academia, industry, and government, including the Faraday Institution Multi-scale Modelling project.

Scarcity of skills

AI has become a strategic priority in the UK across a number of sectors, but its effective deployment depends on a workforce with the right capabilities. Current estimates suggest that only 5% of UK manufacturers have implemented AI across their processes, a gap the High Value Manufacturing Catapult is working to close.[50] The Hartree Centre is also working to increase AI-related skills through the Digital & AI Skills Network, which offers training in AI,

[48] White paper: a UK-US exascale computing and AI collaborative programme for battery science. Download on request.
[49] LF Energy - LF Energy Battery Data Alliance Announces the Battery Data Format (BDF): A New Open Standard for Battery Data Interoperability (January 2026).
[50] HVMC - Unlocking the full potential of AI adoption (August 2025).

data science and high-performance computing for businesses and public sector organisations.[51] Sustained investment to increase workforce AI literacy will be critical to avoid future skills shortages.

Trust

The deployment of AI tools across sectors is often constrained by concerns of trustworthiness. A central challenge is the 'black-box' nature of many AI models, which makes it difficult to determine how specific inputs influence model outputs. In battery R&D, this creates barriers to validation, as researchers cannot easily verify whether predictions reflect physically meaningful relationships or spurious correlations. This is likely to shape the pace of adoption, which may be faster for low-risk, easily cross-checked roles such as literature analysis but slower for safety-critical decisions requiring higher validation and regulatory confidence.

Guidelines and policy have sought to address trust issues in AI more generally. In 2019 the EU published guidelines outlining seven requirements for trustworthiness.[52] Not all of these requirements apply equally to battery-specific applications, given the largely technical rather than personal nature of battery data. Battery-specific research has focused particularly on transparency, with explainable ML offering one route to making AI models easier to understand and validate.[53]

Model validation

AI models can generate predictions, candidate materials or optimised designs rapidly, but these outputs still require experimental or operational validation before they can be relied upon. This validation step remains slow and costly and is often the main constraint on AI's practical impact. This mirrors a wider pattern in AI-enabled science, where a model may identify a promising result in seconds but confirming it experimentally can take weeks or months. The pace of discovery is therefore often governed by validation capacity rather than computational capability, a pattern the Stanford AI Index identifies as a recurring theme across AI-enabled science.[18] Addressing this is not simply a matter of improving model accuracy but also of investing in the infrastructure, protocols and expertise needed to test AI outputs at the pace they are generated.

Infrastructure

Access to the computational infrastructure required to operate AI is a critical challenge. Training and running advanced AI models require substantial compute, data storage and specialised hardware, creating a barrier for research groups and organisations without access to high-performance computing. Sustained investment in this shared infrastructure, rather than in AI models alone, will be necessary to ensure battery researchers can take advantage of increasingly compute-intensive AI methods.

This is reflected in growing UK policy attention, with the government's AI Opportunities Action Plan setting out measures to expand the UK's domestic computing capabilities.[54] Isambard-AI, launched at the University of Bristol in July 2025 with £225 million of government investment, is the UK's largest AI supercomputer, with materials for clean energy among its named use cases.[55] In addition, initiatives such as the NREL-Hartree-Faraday Institution exascale computing collaboration reflect efforts to pool infrastructure across institutions.[48]

Batteries are also playing a growing role in enabling the wider adoption of AI across both industrial and digital infrastructure, particularly data centres.[56] As AI workloads increase the level and variability of electricity demand, batteries are being deployed to provide backup power, smooth peak loads, and improve overall grid resilience. In this way, batteries sit at the intersection of physical AI deployment and digital computing infrastructure, acting as a critical enabler of both operational reliability and scalable AI growth.

Culture

Even where the necessary tools, data and expertise exist, AI adoption can stall if organisations treat it as a peripheral initiative rather than integrating it into core processes. Achieving this integration requires sustained leadership commitment, clear communication of AI's value and limitations, and a tolerance for the iterative, sometimes uncertain nature of early-stage AI deployment. Successful adoption depends on organisational commitment as much as technical capability.

UK policy initiatives supporting AI adoption

The UK government is beginning to take action to support the deployment of AI across science, innovation and manufacturing. The UK government published a new blueprint for AI regulation in October 2025, taking a pro-innovation approach focused on regulating how AI is used rather than the technology itself.[57] The proposed 'AI Growth Lab' would allow AI systems to be tested in controlled environments where certain rules could be temporarily relaxed under strict supervision. This approach is intended to help accelerate the deployment of AI across healthcare, housing and transport, while maintaining safety, trust and regulatory oversight.

Other initiatives include the UK's AI for Science Strategy, launched in November 2025, which directs up to £137 million from a broader £2 billion AI investment towards AI-enabled scientific advances, with materials science explicitly identified as a priority area.[58] It will focus on building high-quality, AI-

[51] Hartree Centre STFC - Digital & AI Skills Network.
[52] European Commission - Ethics guidelines for trustworthy AI (April 2019).
[53] M. Faraji Nri et. al., A Review of the Applications of Explainable Machine Learning for Lithium–Ion Batteries: From Production to State and Performance Estimation, Energies, 2023.
[54] Department for Science, Innovation & Technology - AI Opportunities Action Plan (January 2025).
[55] University of Bristol - UK's most powerful supercomputer launches in Bristol (July 2025).
[56] Battery Council - The batteries behind AI and U.S. data centres (November 2025).
[57] Department for Science, Innovation and Technology - New blueprint for AI regulation could speed up planning approvals, slash NHS waiting times, and drive growth and public trust (October 2025).
[58] Department for Science, Innovation and Technology - AI for Science Strategy (November 2025).

ready datasets through improved standardisation, metadata practices and shared research infrastructure, recognising that a lack of coordination between data sources is a key bottleneck. On skills, the strategy prioritises interdisciplinary capability, bringing together computer scientists, data engineers and domain experts to ensure model validity, alongside upskilling to bridge modelling and experimental science. On autonomous laboratories, the UK's Sovereign AI Unit launched an open call in November 2025 for teams seeking to build unique UK capability, with successful applicants potentially receiving preferential access to national computing infrastructure, alongside investment and technical collaboration.[59] Google DeepMind meanwhile announced it will open its first materials discovery laboratory in the UK in 2026, working with the UK government, with batteries among the named application areas.[60]

The Sovereign AI Fund is a UK government-backed £500 million venture fund designed to strengthen domestic AI capability by investing in British AI startups and infrastructure. It provides firms with capital, access to national compute resources, talent support and government partnerships to help AI companies scale within the UK.[61] In July 2026, the fund co-invested in Cambridge-based CuspAI's $450 million round, valuing the company at $2.6 billion.[4]

Further initiatives are being coordinated through research and industry organisations. The Materials 4.0 Framework addresses the challenges of integrating AI and other technologies into materials science (Box 8). In addition, the Advanced Propulsion Centre's Electrical Energy Storage Roadmap highlights AI as a key enabler of battery innovation acceleration, stating that AI is not a standalone tool but part of a digital system supporting battery production and intelligent monitoring.[62]

Box 8: The National Framework for Materials 4.0

Materials 4.0 is a framework led by the Henry Royce Institute that sits within the National Materials Innovation Strategy, applying the ideas from Industry 4.0 (digitalisation, automation and AI) to materials science and engineering.[63] The aim is to digitally transform the UK's materials science sector by integrating data, computation and automation across the entire lifecycle to transform how materials are discovered, developed, manufactured and deployed. At its core, the framework connects four traditionally separate domains:

- Computational modelling
- Experimental research (including high-throughput and automated labs)
- Data infrastructure (databases, standards, interoperability)
- AI and ML (for prediction, optimisation and inverse design)

These elements are linked in self-driving laboratories in which models propose new materials, automated experiments validate them and the results are used to improve the models. The framework builds on earlier ideas such as the Materials Genome Initiative, but with stronger emphasis on real-time data integration across R&D and manufacturing. Materials 4.0 aims to substantially reduce materials development timelines from decades to years or less, improve reproducibility, and enable more targeted design of materials for specific applications such as batteries, semiconductors and structural alloys.

Conclusions

AI is already being deployed across the whole battery value chain, from materials discovery to cell design, manufacturing and diagnostics. It is not a single technology but a broad toolbox of distinct approaches at different stages of maturity, from well-established predictive modelling through emerging AI-assisted workflows, to early-stage autonomous experimentation. AI has already demonstrated its capability in accelerating scientific discoveries, improve R&D productivity and manufacturing, making it an increasingly critical capability for future innovation across battery research, innovation and manufacturing.

Capturing this potential is not automatic. Wider adoption depends on addressing a set of interconnected challenges spanning data, skills, trust, validation, infrastructure and organisational culture. Strategic choices will also shape the value AI ultimately delivers. Rather than focusing solely on the optimisation of existing chemistries and processes, AI must also be leveraged to identify and develop next-generation materials and advanced manufacturing processes. Lithium-ion cell production remains heavily concentrated in a small number of countries, and the UK's ability to develop competitive, next-generation chemistries will depend in part on how effectively it capitalises on its own strengths, including academic research and innovation.

To support the responsible and effective adoption of AI in battery R&D and manufacturing, the following strategic actions are recommended:

- Invest in data capture, expand computing facilities and improve access to computing resources across battery R&D, recognising that AI is highly dependent on the quality and volume of data.
- Support the development of standardised testing and experimental protocols, metadata and traceable processes for collecting and managing data.
- Rebalance investment across the battery innovation process to include AI-enabled smart synthesis, intelligent

[59] Department of Science, Innovation & Technology - Sovereign AI Open Call: Autonomous Labs (preliminary market engagement) (November 2025).
[60] Silicon republic - Google DeepMind to open UK research lab for discovery of new materials (December 2025).
[61] Sovereign AI.
[62] APC Knowledge Base: Electrical Energy Storage.
[63] Henry Royce Institute - Materials 4.0.

experimentation, testing and at-scale manufacturing optimisation.

- Support AI solutions that improve trust, interpretability and model validation, particularly where outputs inform safety-critical or commercially significant decisions.

Alongside these actions, the purpose and limits of AI need to remain clear and realistic. Human expertise is unlikely to become dispensable; rather, its role will shift towards designing, overseeing and validating increasingly capable AI systems. Expectations for AI should therefore be realistic and balanced against established scientific and physics-based methods. With targeted investment in skills, data infrastructure, computing capacity and standardisation, AI can become a powerful enabling capability for battery innovation. Used effectively, it can accelerate R&D, improve manufacturing and strengthen the UK's position in advanced battery research and industry.

Glossary of terms

Term	Description
Active learning	An iterative loop where the most informative experiments are selected using acquisition criteria such as uncertainty or expected improvement. This reduces experimental cost and accelerates calibration and design.
Agentic AI	Agentic AI systems combine AI models with planning and decision-making capabilities to autonomously execute multi-step tasks using tools and external systems. In battery research, they are being explored to automate workflows although deployment remains early-stage.
Closed-loop optimisation	Closed-loop optimisation refers to a process in which data from experiments, simulations or real-world operation is continuously fed back into models or decision-making systems to improve future outcomes.
Compute	The processing power, memory and storage required to train and run AI models. Increasingly compute-intensive methods, such as large-scale generative models, depend on access to high-performance computing infrastructure, including GPUs, TPUs and data centres.
CPU (Central processing unit)	The main processor in a computer, designed to handle a wide range of tasks and instructions. CPUs are used for general computing, including running operating systems, software and data processing tasks.
Deep learning	Deep learning is a type of machine learning that uses artificial neural networks to learn complex patterns directly from data, enabling applications such as image recognition, language processing, and materials discovery.
Diffusion models	A class of generative AI models that create new data, such as candidate molecular or crystal structures, by learning to reverse a process of gradually adding noise to training data. Diffusion models have become a leading approach for generative materials design due to their ability to handle complex data and incorporate physics-informed constraints.
Digital twin	A digital twin is a virtual representation of a physical system that is continuously updated with real-world data, enabling its behaviour to be monitored, simulated and optimised in real time.
Foundational models	A foundational model is a large-scale AI system that serves as a versatile base layer that can be easily adapted, fine-tuned, or prompted to perform a wide variety of specific downstream tasks.
Generative AI	Generative AI models learn patterns from existing data and use them to create new, similar outputs. In battery research, they are used to propose new material candidates, augment limited datasets, and explore design spaces where experimental data is sparse or costly to obtain.
GPU (Graphics processing unit)	A processor originally designed for rendering graphics, but now widely used for AI and scientific computing as it can perform many calculations in parallel. GPUs are effective for training ML models and processing large datasets.

Term	Description
Knowledge graphs	A knowledge graph links real data into an interconnected network of entities and relationships enabling more intuitive querying, integration and reasoning across datasets.
Large language models (LLMs)	AI models trained on very large text datasets to understand and generate human-like language. LLMs can be used for tasks such as summarisation, coding, technical writing, data analysis and conversational interfaces.
Machine learning (ML)	Machine learning methods use statistical algorithms that learn relationships directly from structured data to make predictions or classifications. In battery research, it is widely used to model state-of-health, predict cycle life and optimise manufacturing processes based on experimental and operational datasets.
Ontologies	An ontology defines the key concepts, entities and relationships within a domain, providing a shared, machine-readable vocabulary curated by human experts.
Physical AI	Physical AI embeds intelligence directly into physical systems, allowing sensing, processing and decision-making to occur in real time within the system itself.
Physics-informed AI	AI models constrained by conservation laws, partial differential equations or physical symmetries to ensure solutions remain physically realistic. These constraints improve learning under sparse data conditions and enhance extrapolation beyond existing datasets.
Reinforcement learning	A machine learning approach in which an AI agent learns to make sequential decisions through trial and feedback, adjusting its strategy based on rewards or penalties to improve long-term performance. In battery research, it has been explored for tasks such as fast-charging protocol optimisation and real-time process control.
Supervised learning	A machine learning approach in which a model is trained on labelled data — known input-output pairs — to learn a mapping it can then apply to new, unseen inputs. Most predictive battery models, such as state-of-health estimation trained on historical cycling data, use supervised learning.
TPU (Tensor processing unit)	A processor developed specifically for ML and AI workloads. TPUs are optimised for the mathematical operations used in neural networks, enabling faster and more energy-efficient AI training and inference in some applications.
Unsupervised learning	An ML approach in which a model identifies patterns or groupings within unlabelled data. In battery research, this can support identifying degradation patterns or materials clusters without predefined categories.
XAI (Explainable AI)	A set of methods and tools designed to make AI systems more transparent and understandable to human users. XAI helps explain how models make decisions, improving trust, interpretability and accountability in AI-driven applications.

About the Faraday Institution and Faraday Insights

The Faraday Institution is the UK's independent institute for electrochemical energy storage research, skills development, market analysis, and early-stage commercialisation. We bring together academics and industry partners in a way that is fundamentally changing how basic research is carried out at scale to address industry-defined goals.

Our 'Faraday Insights' provide an evidence-based assessment of the market, economics, technology and capabilities for energy storage technologies and the transition to a fully electric UK. The insights are concise briefings that aim to help bridge knowledge gaps across industry, academia and government. If you would like to discuss any issues raised by this Faraday Insight or suggest a subject for a future Insight, please contact Stephen Gifford. Sign up today to be added to the distribution list for future Faraday Insights.

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CONTACT
Stephen Gifford
Chief Economist
stephen.gifford@faraday.ac.uk
www.faraday.ac.uk
01235 425125
07741 853068

Dr Mona Faraji Niri
WMG, University of Warwick
mona.faraji-niri@warwick.ac.uk

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