



# A National Framework for Materials 4.0

Pathways to Implementation

ROYCE

April 2026



## **A National Framework for Materials 4.0: Pathways to Implementation**

doi: 10.5281/zenodo.19820031

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April 2026

# Foreword

**The UK stands on the cusp of a profound transformation in how we discover, develop, manufacture, deploy and reuse materials.**

The National Materials Innovation Strategy (NMIS) has already highlighted the central importance of digitally enabled materials innovation in securing the UK's long-term scientific and industrial competitiveness. At the Henry Royce Institute, we have taken this mandate seriously. Over the past two years, we have worked with partners across academia, industry and government to co-develop a National Framework for Materials 4.0, a framework that sets out the digital and data foundations required to accelerate materials innovation and to connect it more effectively to industrial value and national priorities.

Materials 4.0 is already emerging at pace in the UK. Work stimulated through the Government's AI for Science programme is already demonstrating the power of AI-driven approaches for materials discovery, modelling and process optimisation. Our national research community is contributing to a growing body of AI-for-materials capability, from generative design of alloys and composites to intelligent interpretation of microscopy, spectroscopy and complex characterisation data. These advances are vital, but they represent only one strand of the much wider Materials 4.0 landscape. True transformation requires not just powerful models, but the infrastructure, standards and workflows that allow data, tools and models to be accessed, connected and trusted across the full materials lifecycle.

This is why the development of accessible, interoperable and well-governed materials data is paramount. Fragmented, inconsistent or inaccessible data slows innovation, prevents reuse of knowledge, and increases the cost and risk of deploying new materials. Whether in developing the next generation of high-strength steels, scaling advanced composites, building resilient battery supply chains, or assuring long-life performance in aerospace, energy and infrastructure, the ability to link data from discovery through manufacture, into service and ultimately into reuse or recycling is essential. Materials 4.0 creates this "digital thread", not through centralisation, but through federated, standards-based approaches that allow organisations to retain control of their data while still contributing to a coherent national capability.

The benefits are clear. Better data and interoperable tools accelerate discovery, shorten design cycles, reduce non-conformance and waste, improve qualification and certification pathways, and enable more sustainable circular material flows. They support sovereign capabilities in sectors where safety, reliability and traceability are paramount. And they help position the UK as an attractive partner for international collaboration and investment in advanced materials.

This report presents the next stage in building a robust national framework for Materials 4.0. It identifies the infrastructure, standards, governance models and skills required, and sets out a set of practical, evidence-based implementation pathways. Most importantly, it reflects the needs and insights of the UK materials community, which has engaged enthusiastically in shaping a shared national direction.

Realising this vision will require sustained commitment, from government, research institutions, standards bodies and industry. The Henry Royce Institute will continue to convene this community and to champion the investments, skills and partnerships needed to ensure the UK leads in this new era of materials innovation.

Materials 4.0 is not simply an upgrade to existing practice. It is a national capability, essential to our industrial competitiveness, scientific excellence and resilience. The opportunity is immense and now is the time to seize it.

**Professor David Knowles FEng, FIMMM  
CEO, Henry Royce Institute**

# Executive Summary

Materials 4.0 is the data and digital thread through innovation processes. It is a key cross-cutting priority for enhancing the economic and technical potential of materials innovation in the UK. Royce has developed a national framework to support policymakers, research and industry to advance these capabilities.

This framework:

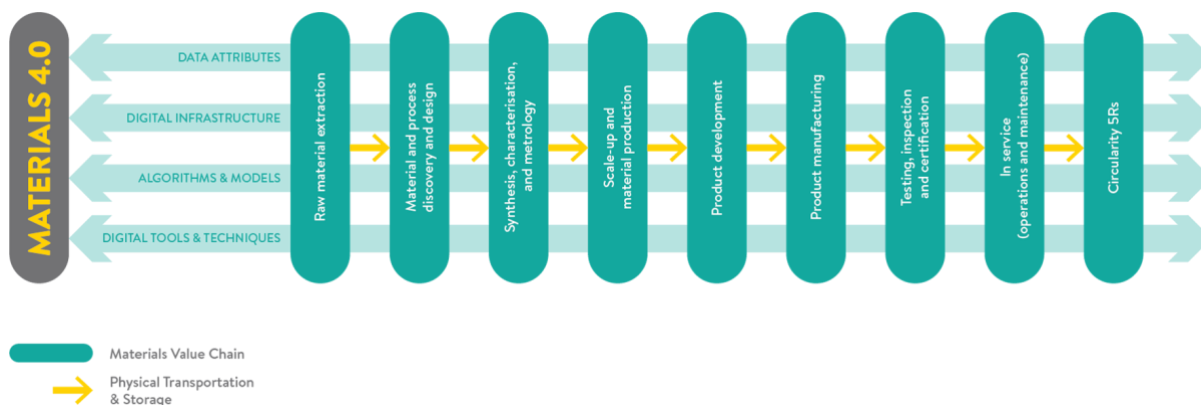
- Provides a common definition of Materials 4.0.
- Defines the economic and technical potential of Materials 4.0.
- Ensures that capability progress evenly across the Materials 4.0 landscape.
- Guides prioritisation and decision-making.

This report features the findings of the second phase of this framework's development, and follows on from the phase 1 report, which can be found on [Royce's website](#).

## The Materials 4.0 framework

The framework is built across two dimensions:

- the materials processes that take place across a material's lifecycle to derive value from it, and
- the digital elements that constitute an ecosystem of data and digital processes across the value chain.



This research has progressed the definition of all four digital elements of the framework to support future adoption and development:

### Data attributes

Data attributes encompass the descriptive and governance characteristics that define material data and its context throughout the materials value chain.

This report presents the Materials 4.0 Data Model (M40DM), which is informed by a review of many existing material ontologies. The model includes the high-level classes

and entities. It highlights how data attributes can be employed, extended and repurposed across a broad range of materials-related contexts and organisations.

### **Digital infrastructure**

Digital infrastructure is the enabling layer that makes connected, governed and reusable materials data possible across a distributed ecosystem.

This framework defines Materials 4.0 Digital infrastructure across four capability areas: Data storage and representation, exchange and execution of data and models, secure connectivity and control, and trust, governance and lifecycle. Together, these infrastructure capabilities enable the digital thread: linking materials information from discovery through manufacture into use and circularity without forcing inappropriate centralisation.

### **Algorithms and models**

Materials data becomes valuable when it is transformed into information, knowledge and actionable decisions. In Materials 4.0, this transformation is achieved primarily through algorithms and models: computational methods that extract meaning from measurements and simulations, learn or encode relationships, support optimisation and decision-making, and provide assurance across the materials value chain.

The algorithms and models used in Materials 4.0 play different roles in turning materials data into useful evidence and decisions. Together, these methods span the progression from preparing and structuring raw data, through predicting and explaining materials behaviour, to supporting optimisation, automation and assurance. All of these roles need to be developed and integrated to generate value from materials data.

### **Digital tools and techniques**

Digital tools and techniques are the operational and user-facing systems that make Materials 4.0 usable in practice. They span the categories of: capture and experiment, data flow and traceability, operational modelling and decisions, and connected physical systems.

Operationalising Materials 4.0 is the point at which digital capability becomes embedded in organisations across the value chain. The key issue at this stage is not only whether data, models and infrastructure exist, but whether they can be integrated into workflows, interfaces and decision processes in forms that are usable, trusted and relevant to researchers, engineers and manufacturers.

## **The potential value of Materials 4.0**

Innovative and strategically significant UK businesses derive substantive and growing commercial value from investment in materials data, models and digital tools.

Industry representatives unanimously agreed that materials properties, performance and data are already integral to directly underpin commercial operations performance, whether through product performance, process efficiency, compliance, lifecycle assurance or end-of-life recovery and that they are expected to become an increasingly significant commercial differentiator in the artificial intelligence age.

Across a broad cross-section of the material sector, including metals, composites, polymers, batteries, biomedical materials and recycling, businesses described

numerous benefits to Materials 4.0 activity, spanning faster product development, lower testing and process costs, stronger traceability and compliance, improved in-service decision-making, and higher-value recovery at end of life.

The commercial significance of Materials 4.0 is clearly conveyed in high demand for materials-related research and innovation projects, of which there have been nearly 6,000 since 2005.

Across the materials value chain, reported benefits of Materials 4.0 include:

- Faster development and time to market, through reduced testing, better use of modelling and more efficient product development.
- Lower cost and improved process efficiency, by reducing waste, avoiding failure events and improving manufacturing and testing productivity.
- Stronger safety, compliance and traceability, through better quality assurance, regulatory evidence and confidence in material provenance.
- Improved in-service performance and decision-making, by linking materials data to inspection, operational and lifecycle information.
- Higher-value circularity and recovery, through better end-of-life visibility and more informed reuse, repurposing and recycling decisions.
- Greater supply-chain resilience and market access, by supporting transparency, accountability and readiness for customer and international regulatory requirements.

These benefits contribute to a UK economy with accelerated innovation cycles, higher industrial productivity, sovereign and resilient supply chains, internationally competitive digital capabilities, and access to growing global markets in critical sectors.

#### Materials 4.0 examples

- Digital passports that trace the critical minerals used in batteries to effectively recover them at the end of its operating life, reducing demands on mining and extraction.
- Programmes that digitally design and test new composite materials, without long physical trial-and-error cycles, accelerating the discovery of new structural capabilities and the components needed for our green energy sector.
- Computational modelling of the lifetime performance of steels used in nuclear components, drastically extending the lifetime of critical assets with reliable insight into their safe operation.

## Priority action plans

There are pervasive barriers to the wholesale development and adoption of Materials 4.0. This framework activity has identified four priority cross-sector challenges that need to be addressed through focussed, coordinated effort.

### Priority 1: Availability of high-quality data

Valuable materials data is often hard to find, inaccessible, poorly described, difficult to exchange between organisations, or locked in legacy systems.

**Action:** Support organisations to generate, manage and share materials data in ways that are consistent, proportionate and reusable, while recognising that different materials, processes and use cases require different levels of structure and detail.

### Priority 2: Incentivising uptake

Investment in Materials 4.0 activity is already taking place across the UK, but capability remains uneven and adoption is still at an early stage in many parts of the materials community.

**Action:** Use public support, incentives and practical delivery mechanisms to help organisations adopt Materials 4.0 approaches in operational settings, building skills and overcoming cultural differences, while coordinating effort at sector level where this can reduce future barriers to entry.

### Priority 3: Data interoperability

Even where materials data exists, it is often difficult to combine, exchange or reuse because definitions, ontologies, formats and software tools are inconsistent.

**Action:** Enable materials data, software tools and digital workflows to work together across organisational and lifecycle boundaries through shared semantics, interoperable standards and federated approaches to connectivity.

### Priority 4: Security and governance

Supply chain actors are protective of certain materials data that they hold. Formulations and processing histories are protectable IPR, and they do not want to share this data in systems that could expose it to competitors.

**Action:** Create the enabling processes and secure collaboration environments needed for supply chain actors to confidently share their valuable materials data with partners.

### Next steps

Materials 4.0 is a strategic capability for the UK, central to productivity, industrial resilience, and scientific leadership. It is critical to realising the national materials innovation strategy and maintaining the UK's leadership in the global materials sector.

The UK has the foundations to lead but requires decisive action across four priorities. Suggested actions and activities for addressing these priorities are provided in this report.

Acting on these priorities now will ensure that the Materials 4.0 national framework delivers across the entire innovation supply chain, from fundamental research to industrial deployment and circular recovery, strengthening national competitiveness for the decades ahead.

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# Introduction to Materials 4.0

**Materials 4.0 is the digital backbone of materials innovation. The structured and comprehensive introduction of Materials 4.0 tools and practices will accelerate and transform materials innovation in the UK and globally.**

Digital and data capabilities mean that the critical minerals in batteries can be traced, creating a new wealth of information on materials that are in-use and could be reused, reducing the demands on mining and extraction. New composite materials can be designed by digital models, unlocking new structural capabilities in the components needed for our green energy sector. The performance of steels in nuclear equipment can be digitally monitored, drastically extending the lifetime of critical assets with reliable data on their safety.

This Materials 4.0 framework defines how data attributes, digital infrastructure, algorithms and models, and digital tools and techniques operate and interact throughout the materials value chain. The framework has been developed through a mixed-methods approach employing both quantitative (e.g. literature reviews, text analytics, web-scraping etc.) and qualitative strategies (e.g. interviews, workshops etc.) for data collection and analysis.

The framework is intended to provide the basis for further investment in an essential technology capability that the UK could lead global efforts in. Suggested actions to overcome priority cross-sector challenges foreseen in Materials 4.0 implementation have been generated during the development of this framework.

## Definition of Materials 4.0

The launch of Royce's National Materials Innovation Strategy (NMIS)<sup>1</sup> in the UK highlighted the importance of accelerating innovation in materials for protecting the UK's position in the global science and technology landscape and capturing significant socioeconomic benefits.

Materials 4.0 emerged as a core cross-cutting theme across all sectors (Figure 1). The strategy defined Materials 4.0 as *'an umbrella term for the ongoing transition to a digitally enabled materials sector. This will be underpinned by a materials informatics framework that combines capabilities in materials modelling, large data, AI and machine learning, in silico modelling, manufacturing informatics, and life-cycle simulation'*.

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<sup>1</sup>[https://www.royce.ac.uk/wp-content/uploads/2025/05/Royce\\_NMIS\\_booklet-digital\\_FINAL-SINGLE.pdf](https://www.royce.ac.uk/wp-content/uploads/2025/05/Royce_NMIS_booklet-digital_FINAL-SINGLE.pdf)

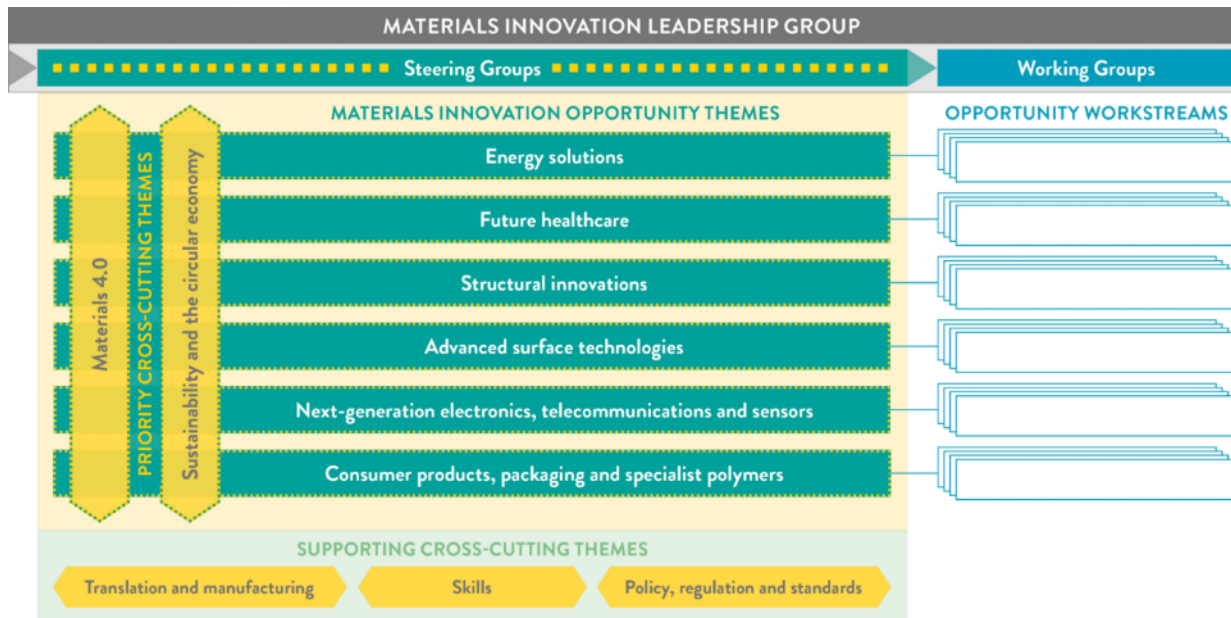



Figure 1. The NMIS implementation plan, which defines Materials 4.0 as a priority cross-cutting theme that will interact with all other innovation workstreams and themes.

## This Materials 4.0 Framework

The purpose of this framework is to provide the basis for the widespread development and adoption of Materials 4.0 in the materials innovation ecosystem and industrial supply chain in the UK. It defines the common structures, practices and languages of Materials 4.0.

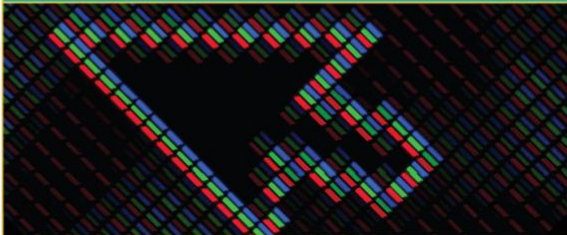
The interim report dealt in detail on the scope and global context of this framework and can be found on Royce’s website<sup>2</sup>. The overarching framework is constructed from two key components:

**Materials Processes**



The steps taken in a materials lifecycle to derive value from it, and where data and digital processes can be applied. These are represented in the framework by vertical discrete elements through which materials are physically transported.

**Digital Elements**



The data and digital ecosystem that wrap around and enable these processes. These are horizontal cross-cutting processes and activities which flow throughout the vertical material value chain elements.

<sup>2</sup> Royce, A National Framework for Materials 4.0 December 2025 Interim Report for Consultation

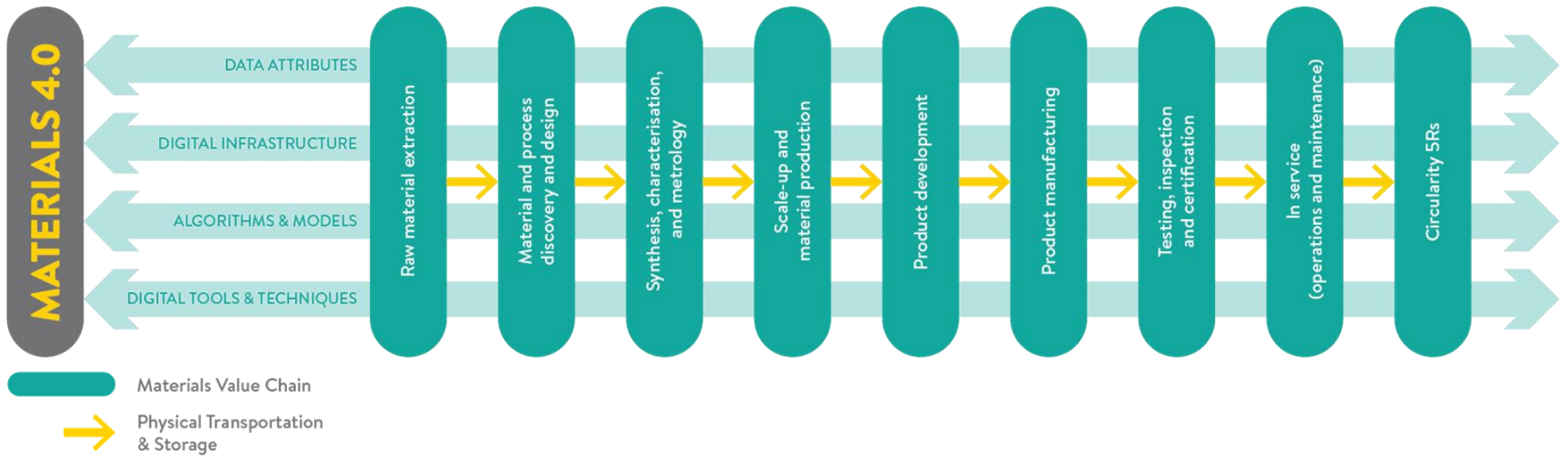


Figure 2: Materials 4.0 across the processes in the materials value chain.

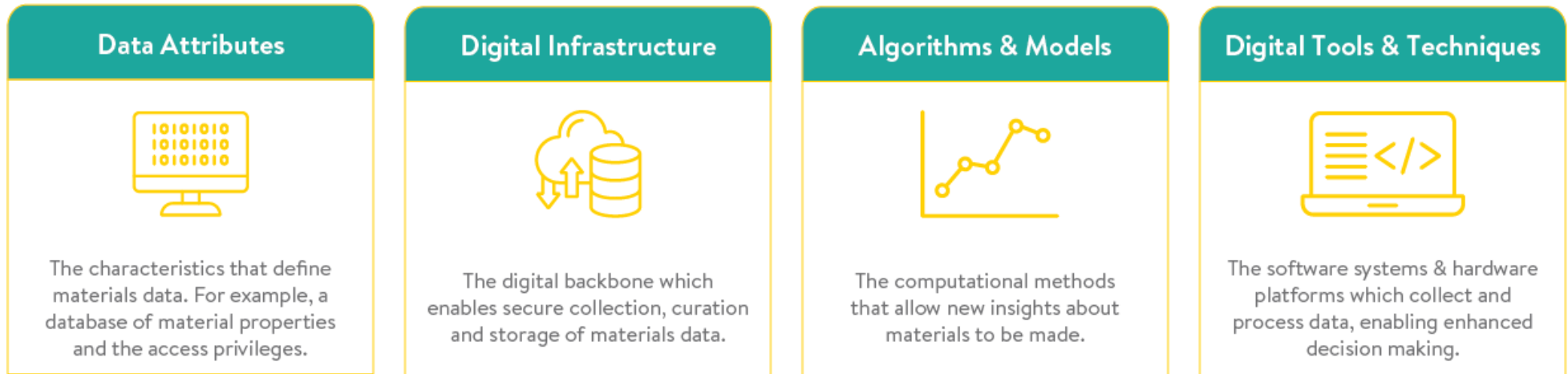


Figure 3: The digital elements of the Materials 4.0 framework.

# The Materials 4.0 Framework

This framework provides a unified approach to Materials 4.0 in the UK. Each of its digital elements have been developed in detail, with a greater focus on the data attributes and infrastructure elements, reflecting the relatively lower investment to date in these areas.

## Data Attributes

Data attributes encompass the descriptive and governance characteristics that define material data and its context throughout the materials value chain.

This include capturing what the data represents, how it is structured, and how it can be accessed, shared, and trusted. Data Attributes are mobilised through interoperable ontologies, compliance with FAIR principles and standards, and supporting metadata for provenance and traceability. The underlying ontology fundamentally shapes the type of data collected, the processes and properties represented and how they relate to each other.

This Materials 4.0 Data Model (M40DM) is informed by a review of many existing material ontologies. The model includes the high-level classes and entities. It highlights how data attributes can be employed, extended and repurposed across a broad range of materials-related contexts and organisations.

### The role of ontologies

Ontologies are universal tools that support data understanding, analysis, sharing, reuse and semantic data management and reasoning.<sup>3</sup> They have been used to drive data stewardship principles such as FAIR data (Findable, Accessible, Interoperable and Reusable).<sup>8</sup>

Ontologies encompass the following key components:

- **Entities:** specific objects within the materials ecosystem to track.
- **Relationships:** links between entities and attributes.
- **Metadata:** contextual details, provenance, and versioning.

Ontologies are usually subdivided into the different levels of abstraction that they operate in, as illustrated in Figure 4. Overall, top-level ontologies are expected to be domain agnostic, covering broad, general concepts to ensure consistency in the definition of basic categories such as objects or processes.

Notable top-level ontologies are the ISO-introduced Basic Formal Ontology and the Descriptive Ontology for Linguistic and Cognitive Engineering (DOLCE) and, for the

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<sup>3</sup> Rajamohan, B. P., Bradley, A. C. H., Tran, V. D., Gordon, J. E., Caldwell, H. W., Mehdi, R., & French, R. H. (2025). Materials data science ontology (mds-onto): Unifying domain knowledge in materials and applied data science. *Scientific Data*, 12(1), 628.

materials science and engineering context the Elementary Multiperspective Material Ontology (EMMO).

Mid-level ontologies on the other hand add more specific entities and relationships, while preserving some degree of modularity, such as the Platform Material Digital Core Ontology (PMDco) that focusses on materials science and engineering.

Low-level ontologies are aimed at a specific field of application, such as the Materials Data Science ontology (MDS-onto) which aims to standardise terminology related to materials data. Domain and subdomain level ontologies are the most specific ones, instantiating and expanding the broader ontologies to target particular applications, products or processes. One example is the Atomistic Simulation Methods Ontology (ASMO) which focusses on describing and standardising simulation methods in materials science.

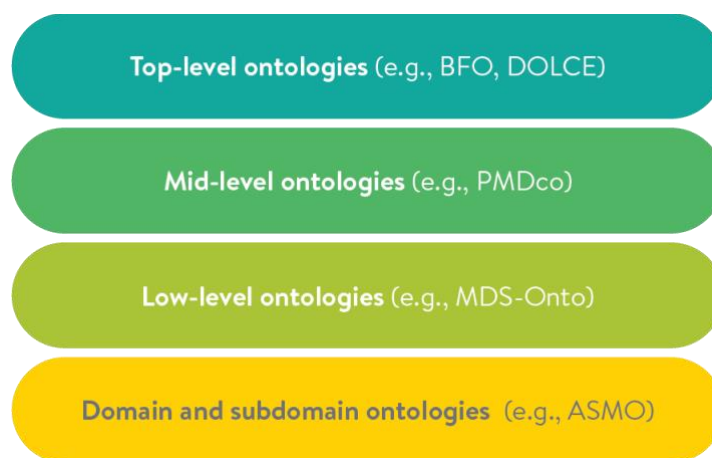


Figure 4. Overview of different ontology levels.

Ontologies' role in structuring data exchange is internationally recognised, which includes a specific ISO standard family to versing about the requirements for top-level ontology development.<sup>4</sup>

While many initiatives to develop ontologies already exist in the materials science and engineering space, they often have limited impact, poor documentation and limited curation and maintenance<sup>5</sup>, hindering their adoption.

### Work-to-date

In Appendix I, an overview of 10 existing material ontologies, data frameworks and standards that are relevant to Materials 4.0 is provided. There is also a detailed international case study on Germany's approach to ontology development.

Germany views semantic infrastructure as a national strategic asset, similar to major research facilities, with significant public funding and coordinated, consortium-based

<sup>4</sup> ISO/IEC 21838-1:2021. Information technology — Top-level ontologies (TLO). Part 1: Requirements.

<sup>5</sup> Bayerlein, B., Schilling, M., Birkholz, H., Jung, M., Waitelonis, J., Mädler, L., & Sack, H. (2024). PMD Core Ontology: Achieving semantic interoperability in materials science. *Materials & Design*, 237, 112603.

programmes. It hosts over 40 initiatives advancing ontologies for materials science and engineering, which fall under three streams:

1. NFDI (DFG-funded): National Research Data Infrastructure programmes.
2. Platform MaterialDigital (BMBF-funded): National effort to digitise materials data and workflows.
3. Independent initiatives: EU-funded and institute-led ontology development projects.

They are all working towards a shared long-term goal to create interoperable materials knowledge ecosystems that make data more findable, searchable, and shareable across institutions and disciplines.

### The Materials 4.0 Data Model (M40DM)

Ontologies structure data in ‘machine-understandable’ representations of a domain<sup>6</sup>. An ontology consists of **classes** (sets of instances that share common characteristics e.g. ‘material’ or ‘process’), **properties** (the relationship between instances or the relationship between an instance and a data value e.g. usesResources or hasNumericValue), and **constraints** (restrictions on how classes and properties may be used e.g. numeric values must be xsd:decimal).

Each ontology deals with different levels of granularity of information. For this study, ten different material ontologies were reviewed, mainly at mid-level. In total, 34 different classes were identified and consolidated into the high-level classes that could be used to develop an example Materials 4.0 Data Model (M40DM), as shown in Figure 5.

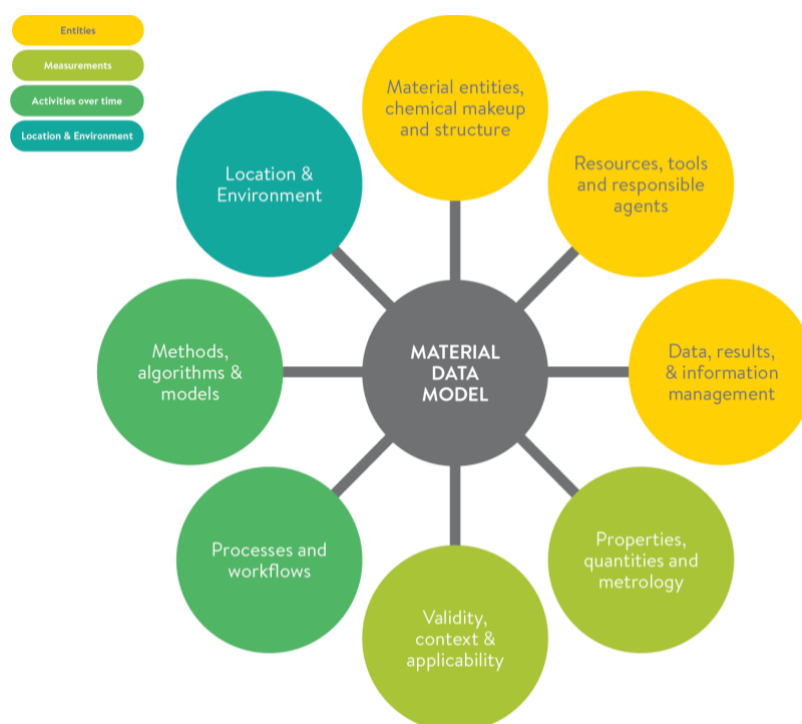


Figure 5: Schematic of the Materials 4.0 Data Model

<sup>6</sup> ‘Digitalizing Material Knowledge: A Practical Framework for Ontology-Driven Knowledge Graphs in Process Chains’ <https://doi.org/10.3390/app142411683>

The table below details the high-level classes and constituent sub-classes of the Materials 4.0 data model.

Table 1: Detailed high-level classes and sub-classes of the Materials 4.0 Data Model.

High-level class	High-level class Definition	Sub-class	Sub-class Definition
<b>Material Entities, Chemical Makeup and Structure</b>	Physical or chemical entities that are the subject of investigation, design, or processing.	Product / Material System	A defined material or product about which properties and data are claimed.
		Material	A substance or material system (e.g., alloy, polymer, ceramic).
		Sample / Specimen	A prepared or selected material entity used for testing or analysis.
		Atom / Chemical Entity	Chemical constituents defined by external standards (e.g., ChEBI).
		Composition	Description of constituents and their quantitative fractions.
		Physical State	State or phase of the material (e.g., solid, liquid, phase assemblage).
		Structure	How a material is internally arranged or physically characterized. Arrangement of sites, occupancies, or internal organization of a material.
<b>Resources, Tools &amp; Responsible Agents</b>	Entities that enable or perform processes.	Resource	Anything required to perform a process.
		Agent	Person, organization, software)
		Tool / Equipment / Device	Consumable / Material Resource
		Resource Property	Characteristics of a resource (e.g., calibration, capability).
		Process / Resource Representation	Documentation or models describing resources or processes.
<b>Data, Results &amp; Information Management</b>	Information artifacts produced, exchanged, and referenced.	Data / Results / Outputs	Datasets, files, records, reports, model outputs.
		Identifier / Reference	Persistent identifiers (URI, DOI, internal ID).

		Product / Material Definition & Classification	Formal definition and classification references.
<b>Properties, Quantities &amp; Metrology</b>	What is claimed or measured about a material and how it is expressed.	Fundamental property	An intensive physical property of a material that does not depend on the amount of the material. An intrinsic trait of a material/entity that can be described or measured (e.g., band gap, hardness, etc.)
		Emerging / Engineering property	A contextual trait of a material/entity that can be described or measured. It depends on where/how a material is made.
		Property Value	The value of a property (scalar, array, or function).
		Quantity	A measurable property value.
		Unit	Standard measurement unit (QUDT-compatible).
		Uncertainty / Quality Metadata	Level of errors due to purity, defects, contaminants etc. Accuracy, tolerance, confidence, or error associated with values.
<b>Validity Context &amp; Applicability</b>	The conditions under which a property value or result is valid.	Data Environment / Validity Conditions	Experimental, operational, or computational parameters affecting results.
		Effectivity	Time range, configuration, batch, or applicability scope.
<b>Processes &amp; Workflows</b>	Activities that act on entities over time.	Process	Any operation that transforms, measures, or analyzes entities.
		Measurement / Observation	A process that determines property values.
		Pre-processing	Setup, calibration, tolerances, specimen preparation.
		Post-activity Processing	Surface treatment, coating, finishing.
		Data Post-processing	Transformation or analysis of raw outputs.
		Process-Product Linkages	Explicit relations: acts-on, produces, determines, consumes.

<b>Methods, Algorithms &amp; Models</b>	Specifications describing <i>how</i> processes are carried out.	Method Protocol	/	Prescribed experimental or procedural specification.	or
		Algorithm		Formal computational procedure.	
		Model Simulation	/	Conceptual, mathematical, or computational representation.	or
<b>Location &amp; Environment</b>	Where entities or information are situated.	Physical Geospatial Location	/	Laboratory, facility, site, or geographic place.	
		Information Location		File path, database entry, table row/column.	

Important data principles such as Findability, Accessibility, Interoperability, and Reusability (FAIR), standards, data ownership, data security, data sharing, data governance, data structures, data quantity, data quality, data trust, and data traceability are encompassed by all the high-level classes and are fundamental to the material data model.

Furthermore, the eight high-class elements can be sequenced in a relations diagram as shown in Figure 6.

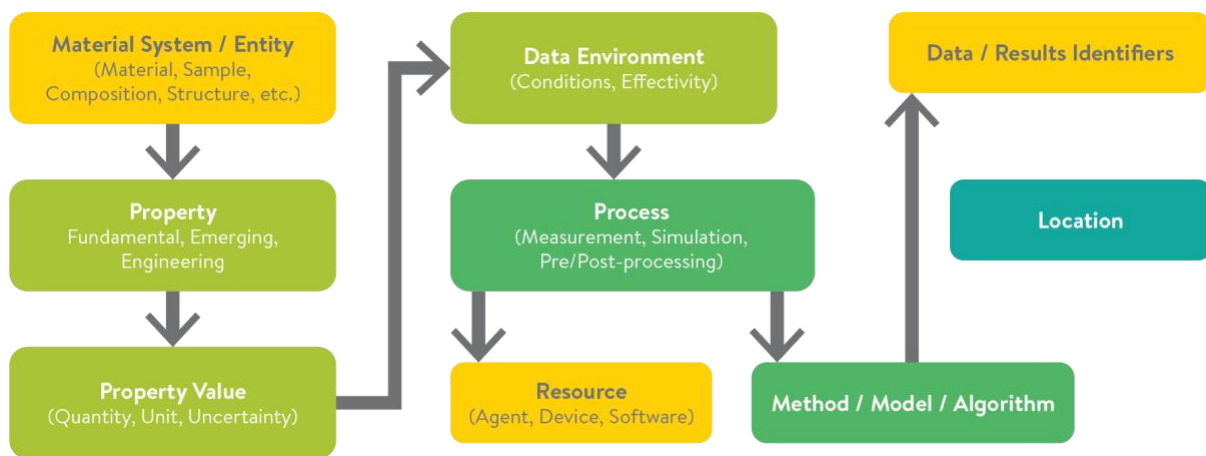


Figure 6: Relations diagram between the eight high-class elements constituting the Materials 4.0 Data Model

# Digital Infrastructure

Digital infrastructure is the enabling layer that makes connected, governed and reusable materials data possible across a distributed ecosystem.

Its role is to provide the technology needed for data storage, computation, interoperability, secure exchange and trust mechanisms needed for a digital thread spanning research, manufacture, use and circularity.

Table 2: The digital infrastructure capability areas required for Materials 4.0.

Data storage and representation	Exchange and execution of data and models	Secure connectivity and control	Trust, governance and lifecycle
<p><b>Structured databases and knowledge graphs</b></p> <p><b>Role:</b> Store high-integrity materials records and relate materials, processes, properties and evidence for traceability and complex querying.</p> <p><b>Example:</b> Databases hold batches, test results and specifications, while knowledge graphs connect these records across value-chain contexts.</p>			
<p><b>APIs and interoperability layers</b></p> <p><b>Role:</b> Exchange materials data in consistent, machine-readable forms so tools and organisations can work together without document-based handoffs.</p> <p><b>Example:</b> An industrial tool, repository and modelling workflow consume the same materials data through shared interfaces rather than manual file transfer.</p>			
<p><b>Secure networking and data exchange fabric</b></p> <p><b>Role:</b> Move materials data reliably and in a governed way between instruments, on-premises systems, cloud services and national compute environments.</p> <p><b>Example:</b> Standard protocols, encrypted transfer, network segregation and high-throughput gateways support secure movement of large imaging and characterisation datasets.</p>			
<p><b>Cloud and edge computing architectures</b></p> <p><b>Role:</b> Provide the execution environment for data capture, processing, analytics and model development/execution, from local low-latency edge compute to scalable cloud and HPC resources.</p> <p><b>Example:</b> Edge systems support local capture close to equipment, while cloud or HPC environments run intensive analytics and model execution at scale.</p>			
<p><b>Governance, lifecycle and trust controls</b></p> <p><b>Role:</b> Keep infrastructure secure, compliant and reliable over long product lifecycles through stewardship, backups, retention, archiving, versioning, access policies and operational monitoring.</p>			

**Example:** Logs, metrics, alerts and audit trails maintain trustworthy systems, datasets and evidence chains across extended materials and component lifecycles.

Together, these infrastructure capabilities enable the digital thread: linking materials information from discovery through manufacture into use and circularity without forcing inappropriate centralisation.

For researchers and industry, the benefit is in reduced friction and lower risk, faster Materials 4.0 development and certification, stronger traceability and evidence retention, controlled sharing across the value chain, and access to robust, scalable compute where complex calculations are needed.

## Existing UK digital infrastructure

The categories above describe the main classes of infrastructure capability that Materials 4.0 depends upon. The underlying digital infrastructure must exist within the UK, but it must also be practically accessible to the materials community if those capabilities are to be realised in practice, particularly where materials data must be shared, governed and computed across organisational boundaries. The following reviews UK digital infrastructure in a context relevant to Materials 4.0.

A major feature of the current UK digital infrastructure landscape is the dominant role of the large cloud hyperscalers, with Amazon Web Services (AWS), Microsoft Azure and Google Cloud Platform (GCP) all maintaining established multi-site UK presences. Each hyperscaler platform offers extensive capability and proprietary tools and approaches that can create a degree of vendor lock-in.

Open standards such as containerisation via Kubernetes and data portability protocols mean that organisations can increasingly build workflows that span multiple providers, reducing dependency on any single hyperscaler and enabling more flexible, resilient data strategies. Research has shown that in practice switching between cloud providers is not prevalent and hybrid use of multiple providers is more common.

There are no credible UK alternatives to the US-headquartered hyperscalers with these organisations investing and outspending all others by orders of magnitude. The European Union has responded to this dependency through initiatives such as GAIA-X<sup>7</sup>, a framework designed to foster interoperable, sovereignty-assured cloud infrastructure across member states.

The practical consequence for UK materials research and industry is a significant degree of reliance on digital infrastructure potentially governed by US law. A UK competition authority review concluding in 2025 found that certain features of the UK cloud services markets lead to adverse effects on competition and highlight technical and commercial barriers within the UK digital infrastructure market<sup>8</sup>.

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<sup>7</sup> Gaia-X: A Federated Secure Data Infrastructure, [gaia-x.eu](https://gaia-x.eu)

<sup>8</sup> UK Competition and Markets Authority, [Cloud services market investigation](#)

The UK government has responded to these gaps through a series of interconnected commitments.

- The AI Opportunities Action Plan, published in January 2025, established a framework covering sovereign compute, public data access, and AI investment<sup>9</sup>.
- The Compute Roadmap, published in July 2025, commits up to £2 billion through to 2030 with an ambition of reaching 6GW of AI-capable data centre capacity nationally<sup>10</sup>.
- The AI for Science Strategy adds a further £137 million directed at research applications, requiring UKRI to ensure experimental data meets FAIR principles by 2030, with repositories co-located with sovereign compute at Bristol and Edinburgh<sup>11</sup>.
- The Data (Use and Access) Act 2025 provides the legislative foundation for more consistent data governance across public and private sectors<sup>12</sup>.
- A dedicated Sovereign AI Unit, backed by up to £500 million, has been established to invest in domestic AI capability, supported by AI Growth Zones designed to streamline planning and energy access for new facilities<sup>13</sup>.

For Materials 4.0, the key implication is that digital infrastructure capability in the UK is substantial, but practical use across research and industry still depends on interoperability, access arrangements, governance and confidence in long-term control of data and compute.

### **A federated model of digital infrastructure for M4.0**

For Materials 4.0, a single monolithic digital infrastructure across the full value chain is neither realistic nor necessarily desirable. It would require extensive coordination across multiple organisations and operational environments, together with sustained long-term collaboration to establish, govern and maintain.

Instead, a federated approach is more agile and flexible. In this approach, organisations across the value chain (e.g., laboratories, test houses, manufacturing, and recyclers) will continue to retain data locally for reasons of IP, cost, performance, and regulation.

Data is shared via a set of mutually agreed interoperability layers, such as shared schemas and identifiers, APIs, metadata services, and identity/access controls, that allow those distributed data assets to be connected and governed as part of a coherent end-to-end digital thread when and where needed. These tools are readily available as flexible off-the-shelf solutions and are in use in other secure data environments, including financial services.

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<sup>9</sup> AI Opportunities Action Plan, [AI Opportunities Action Plan](#)

<sup>10</sup> UK Compute Roadmap, [UK Compute Roadmap](#)

<sup>11</sup> AI for Science Strategy, [AI for Science Strategy](#)

<sup>12</sup> Data (Use and Access) Act 2025. [Data \(Use and Access\) Act 2025: data protection and privacy changes](#)

<sup>13</sup> Sovereign AI Unit, [Sovereign AI Unit - GOV.UK](#)

In a federated model of digital infrastructure, a key architectural idea is to distinguish between where data physically resides and how it is discovered, accessed and linked. This is reflected in four core principles: decentralised data retention, interoperability standards, distributed governance, and a federated access layer. Together, these principles distinguish a federated model from both full centralisation and ad hoc bilateral data exchange, by separating local control of data from shared mechanisms for discovery, access and trust.

A practical Materials 4.0 federated digital infrastructure model across the Materials value chain is shown in Figure 7.

To operationalise this in industrial settings, treat high-value materials data as data products. These are standardised, versioned packages with explicit schema/metadata, provenance, quality assertions and access conditions and the digital infrastructure should be geared to deliver this.

For Materials 4.0, the key infrastructure challenge is likely not to centralise all data and computation into a single system, but to allow organisations to easily create trusted and interoperable environments in which distributed data, models and workflows can be connected when needed. In practice, this points towards federated architectures, shared standards and data-product thinking as the most credible basis for scalable adoption across the UK materials ecosystem.

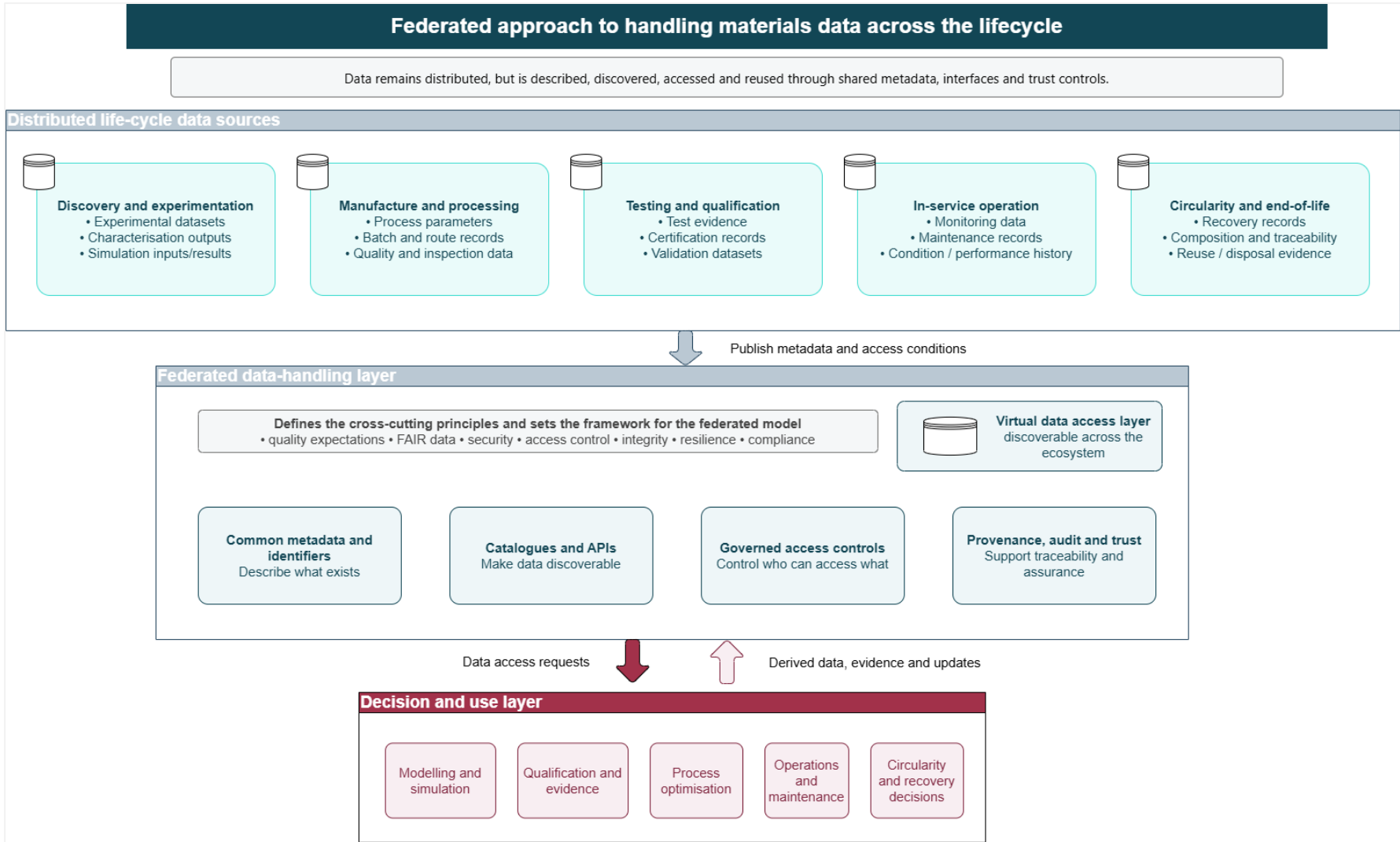


Figure 7: Federated digital infrastructure system use in a material value chain.

# Algorithms and Models

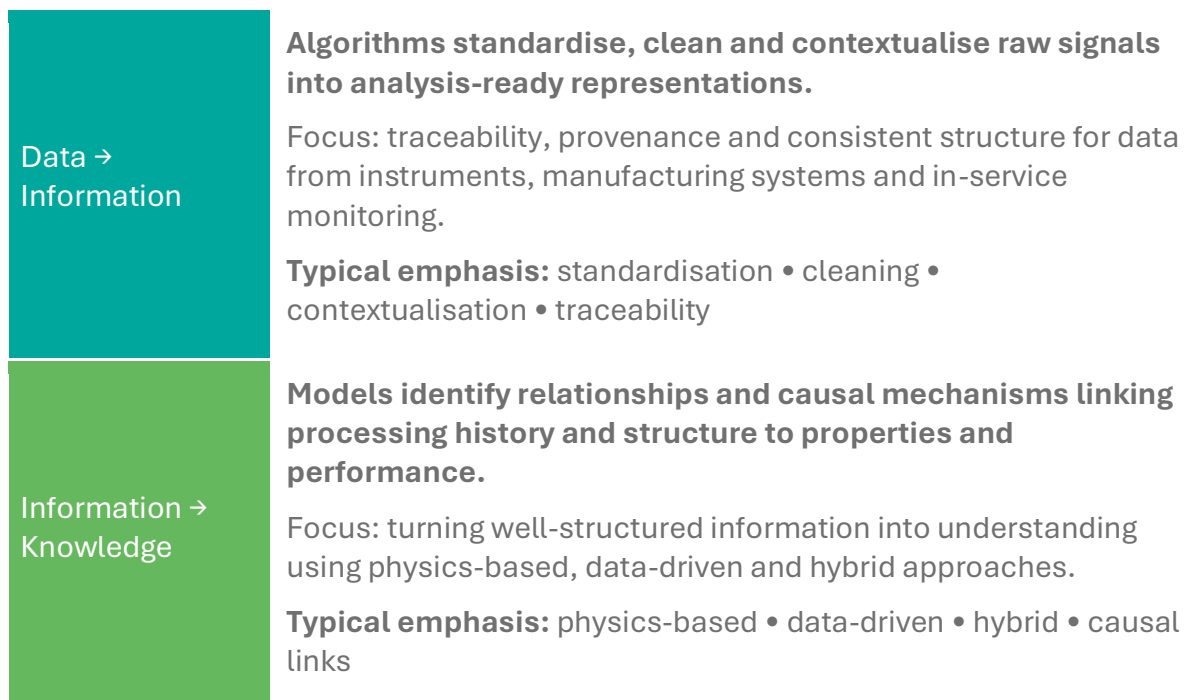
Materials data becomes valuable when it is transformed into information, knowledge and actionable decisions. In Materials 4.0, this transformation is achieved through algorithms and models: computational methods that extract meaning from measurements and simulations, learn or encode relationships, support optimisation and decision-making, and provide assurance across the materials value chain.

In practical terms, algorithms and models connect materials' structure, processing, properties and performance, enabling predictions (what will happen), explanations (why it happens), and prescriptions (what should be done next).

Algorithms and models operate across the Materials 4.0 framework: they depend on robust data attributes and infrastructure, and the outputs are deployed to end users through digital tools and techniques such as simulation environments, analytics platforms and digital twins.

## The role of algorithms and models

Figure 8 illustrates the role of algorithms and models through the data–information–knowledge–wisdom hierarchy. In Materials 4.0, these methods do not serve a single purpose, but play different roles as materials data becomes more decision-relevant. This progression highlights that Materials 4.0 is not simply about collecting more data, but about converting data into increasingly actionable forms of evidence across the value chain. At the point where model outputs begin to inform engineering, qualification and lifecycle decisions, uncertainty quantification becomes essential in judging how much confidence can be placed in those outputs.



Knowledge →  
Wisdom

**Decision methods convert predictions into choices while acknowledging trade-offs, uncertainty and governance constraints.**

Focus: selecting process settings, building qualification evidence, setting inspection intervals and shaping circularity strategies.

**Typical emphasis:** optimisation • uncertainty quantification • decision support • governance

Figure 8: The role of algorithms and models through the data-information-knowledge-wisdom hierarchy

### Main classes of Materials 4.0 lgorithms and models

The algorithms and models used in Materials 4.0 play different roles in turning materials data into useful evidence and decisions. Together, these methods span the progression from preparing and structuring raw data, through predicting and explaining materials behaviour, to supporting optimisation, automation and assurance.

Materials 4.0 does not rely on a single modelling approach, but on a complementary set of methods that operate at different stages of the digital workflow and address different decision needs across the materials value chain.

Table 3: Algorithm and model types, roles and examples.

Data foundation	Predictive models	Decision and automation	Assurance
<b>1. Data processing algorithms</b> <b>Role:</b> Convert raw instrument, image, spectra and process data into standardised, analysis-ready descriptors. <b>Example:</b> Extract grain size and aligned metadata from microscopy, composition and heat-treatment records turning heterogeneous laboratory data into a consistent data product representing material state, which can then be reused			
<b>2. Physics-based models</b> <b>Role:</b> Use physical laws, empirical and phenomenological models to predict material behaviour with strong interpretability and extrapolation. <b>Example:</b> Link alloy chemistry and heat treatment to microstructure, strength and toughness.			
<b>3. Data-driven and ML models</b> <b>Role:</b> Learn patterns from experimental, simulation, manufacturing and in-service data for fast prediction or detection. <b>Example:</b> Predict fatigue strength and classify porosity from XCT imagery for quality triage.			

#### 4. Hybrid models

**Role:** Blend physical structure with data calibration to improve realism, confidence and transferability.

**Example:** Calibrate irradiation and temperature models for nuclear graphite using measured data.

#### 5. Surrogate models

**Role:** Approximate expensive simulations with rapid emulators for design loops, twins and uncertainty studies.

**Example:** Embed a fast steel pressure-vessel response model inside a digital twin for near-real-time forecasting.

#### 6. Optimisation and design algorithms

**Role:** Turn models into decisions by searching composition, process and microstructure trade-offs under constraints.

**Example:** Recommend the next coating formulations to test while balancing hardness, corrosion, cost and manufacturability.

#### 7. Knowledge extraction and understanding from unstructured evidence

**Role:** Use AI and related methods to extract, classify and structure materials-relevant information from reports, certificates, notes and other documentary evidence and provide natural language interfaces to materials information and knowledge in ways that aid interpretation, retrieval and decision-making.

**Example:** Extract chemistry, process route, test conditions and results into a governed schema with human review.

#### 8. Uncertainty quantification

**Role:** Quantify uncertainty in inputs, models and outputs so decisions are based on confidence, not point estimates.

**Example:** Estimate the probability that an additively manufactured aircraft part meets strength and fatigue requirements.

### Implications for Materials 4.0

Analysis indicates that algorithms and models account for around 44% of UK research and investment activity across the materials value chain, and this is a rapidly expanding area as new techniques mature. For example:

- Graph neural networks are used to predict crystal structures and material properties, and are now a core method within computational materials discovery<sup>14</sup>.
- Weld simulation modelling using material-specific properties to accurately predict thermal distribution, structural distortion and residual stresses in welded components<sup>15</sup>. When coupled with lifetime history and operational loading data, this forms a weld-level digital twin that can be used to predict damage accumulation, crack initiation and remaining useful life, and to support inspection, repair and life-extension decisions.
- Hybrid physics-based and data-driven models, including physics-informed neural networks, for problems involving sparse data, multi-scale behaviour and physically constrained systems<sup>16</sup>.
- Large language models are increasingly being explored for extracting structured materials information from the scientific literature, enabling the construction of reusable datasets and knowledge graphs<sup>17</sup>.

The UK's challenge is therefore not a lack of high-quality research or capability in algorithms and models. Rather, activity is often concentrated at early stages of materials discovery and design, with comparatively limited translation of this capability into operational value across manufacturing, qualification and whole-life materials management at industrial scale<sup>18</sup>. As a result, models that show clear promise in research environments frequently struggle to be adopted in practice.

The key implication for Materials 4.0 is the need to shift emphasis from model development alone to model deployment and use in industry. This requires closer coupling between research teams and industrial partners from the early stages of model development, so that models are designed with deployment, integration and assurance in mind. In practice, this means building models that can operate with sparse, noisy and fragmented production data, that integrate with existing digital infrastructure and workflows within company enterprise systems, and that support traceability, validation and confidence in decision-making.

Addressing this gap is critical if the UK is to convert its strong research base in algorithms and models into deployed capability that delivers measurable impact across materials discovery, manufacturing, qualification and lifecycle management.

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<sup>14</sup> For example: [Examining graph neural networks for crystal structures: Limitations and opportunities for capturing periodicity](#)

<sup>15</sup> For example: [Surrogate model development using simulation data to predict weld residual stress: A case study based on the NeT-TG1 benchmark](#)

<sup>16</sup> For example: [Physics-Informed Neural Networks in Materials Modeling and Design: A Review](#)

<sup>17</sup> For example: [Extracting and reconstructing knowledge in materials science literature using large language models](#)

<sup>18</sup> DSIT, [Insights from the UK Innovation Diffusion & Adoption Survey](#)

# Digital Tools and Techniques

Digital tools and techniques are the operational and user-facing systems that make Materials 4.0 usable in practice.

They enable data capture from laboratories and production environments, orchestrate routine workflows and initial processing, and deliver outputs from analytics, models and algorithms back to practitioners in forms that support better decisions and action. This may take the form of recommendations and optimised process settings presented to end users, or fully automated closed-loop operation in which models and algorithms feed directly into in-process control and manufacturing systems without human input.

## Operationalising Materials 4.0

Operationalising Materials 4.0 is the point at which digital capability becomes embedded in organisations across the value chain. The key issue at this stage is not only whether data, models and infrastructure exist, but whether they can be integrated into workflows, interfaces and decision processes in forms that are usable, trusted and relevant to researchers, engineers and manufacturers. This is the layer at which digital capability is translated into day-to-day operational value across the materials value chain.

There is overlap with elements of digital infrastructure, particularly where integrated platforms (such as Databricks or Microsoft Fabric) provide both foundational data services (e.g. data storage, compute provision and access control) whilst enabling operational capabilities (workflow orchestration, analytics execution and dashboarding). In the Materials 4.0 framework, the distinction is best understood in terms of purpose: digital infrastructure enables secure, governed capability at scale, while digital tools and techniques deliver that capability into operational use.

## Main categories of digital tools and techniques

Materials 4.0 depends not only on data and models, but also on the practical tools that embed those capabilities into day-to-day research, engineering, manufacturing and operational decision-making across the value chain.

Table 4: Categories of Materials 4.0 digital tools and techniques.

Capture and experiment	Data flow and traceability	Operational modelling and decisions	Connected physical systems
<p><b>1. Data acquisition and capture tools</b></p> <p><b>Role:</b> Collect and digitise data from instruments, manufacturing equipment and in-service monitoring systems.</p> <p><b>Example:</b> Microscopy, spectroscopy and test-machine outputs are captured with identifiers and metadata through a laboratory management system.</p>			
<p><b>2. Laboratory workflow and experiment management tools</b></p> <p><b>Role:</b> Plan, schedule, record and track experiments so workflows are reproducible, traceable and trusted.</p>			

**Example:** An electronic lab notebook linked to robotic synthesis logs protocols automatically and tracks sample lineage into a shared repository.

### 3. Data pipelines and workflow orchestration tools

**Role:** Move, transform, validate and route data between instruments, repositories and analytical environments.

**Example:** University characterisation data is reformatted to a common schema, quality-checked and exposed to an industrial modeller through an API.

### 4. Lifecycle traceability and product information tools

**Role:** Maintain an auditable record of identity, provenance, process history, test evidence and service data across the value chain.

**Example:** A nuclear steel component record links raw material provenance, manufacturing history, inspection results and in-service condition data.

### 5. Digital twins and simulation delivery environments

**Role:** Connect models and simulations to live or historical data so predictions can be used in real operational contexts.

**Example:** A battery electrode production twin uses in-line sensor data to surface recommended process adjustments before off-spec material is produced.

### 6. Analytics, visualisation and decision-support tools

**Role:** Present processed data and model outputs to the right user in the right form to support practical decisions.

**Example:** Researchers, qualification engineers and fleet managers access the same underlying data environment through role-specific decision views.

### 7. Industrial connectivity, sensing and automation tools

**Role:** Connect physical materials processes and deployed assets to the digital environment through IoT networks, embedded sensors, inspection systems and automated equipment.

**Example:** An offshore wind turbine blade carries inspection history from manufacture, streams strain and acoustic data in service, and passes accumulated condition evidence into end-of-life remanufacture or recovery decisions.

# The Value of Materials 4.0

**Industry consultations conducted to inform this research highlighted clear and growing commercial value from investment in materials data, models and digital tools.**

Across a broad cross-section of the material sector, including metals, composites, polymers, batteries, biomedical materials and recycling, businesses described numerous benefits to Materials 4.0 activity, spanning faster product development, lower testing and process costs, stronger traceability and compliance, improved in-service decision-making, and higher-value recovery at end of life.

While the link between specific data investments and financial return is not straightforward to isolate, the direction of travel is clear: materials data is increasingly being treated as fundamental to competitiveness, resilience and innovation across the materials lifecycle.

More information on this value is provided in Appendix 2.

## Overview of Benefits

**Industry representatives unanimously agreed that materials properties, performance and data are already integral to commercial performance, and that they are expected to become an increasingly significant commercial differentiator in the artificial intelligence age.**

Across the materials value chain, reported wide-ranging and substantive productivity benefits of Materials 4.0 including:

- Faster materials development and reduced time to market, through more efficient materials testing, better use of materials modelling and more efficient product development.
- Lower cost and improved process efficiency, by reducing waste, avoiding failure events and improving manufacturing and testing productivity.
- Stronger safety, compliance and traceability, through better quality assurance, regulatory evidence and confidence in material provenance.
- Improved in-service performance and decision-making, by linking materials data to inspection, operational and lifecycle information.
- Higher-value circularity and recovery, through better end-of-life visibility and more informed reuse, repurposing and recycling decisions.
- Greater supply-chain resilience and market access, by supporting transparency, accountability and readiness for customer and regulatory requirements.

## Investment Activity in Materials 4.0

Business investment in Materials 4.0 activity is already substantial, but often difficult to quantify precisely. Interviewees described significant and growing spend on Materials 4.0 activity, including materials-specific teams, new employment roles and skills, research and development, investment in software, analytical equipment, in-process measurement and wider digital capability.

### Illustrative example: investment in materials recycling

One major UK recycling business described a substantial programme of data, modelling and digital twinning activity targeted at developing new, higher-value forms of recycle. The same business is also investing in a major facility for bulk scrap measurement, illustrating how Materials 4.0 investment combines digital capability and physical infrastructure to deliver benefit across the materials value chain.

Materials 4.0 investment is often embedded across broader programmes in R&D, manufacturing improvement, digital systems and data infrastructure. Examples cited included major expenditure on characterisation equipment, internal investment in data and modelling capability, and growing effort to integrate materials data more effectively into wider business processes.

Public funding was seen as playing an important enabling role in encouraging further Materials 4.0 activity. Interviewees highlighted the value of support for skills development, collaborative R&D and demonstration activity, particularly where organisations are building capability or exploring emerging approaches. This suggests that public support may have an important role in accelerating capability development and helping emerging Materials 4.0 approaches move towards wider industrial use.

### Commercial motivations

According to consultees, the primary commercial drivers for investing in materials data span six interconnected themes:

Accelerated product development and reduced time to market

Materials data, modelling and simulation can reduce testing burden, shorten development cycles and help organisations reach stable designs more quickly.

### Accelerated development in composites

A composite materials developer indicated that design phases for aerospace applications can take over twelve months, while for automotive the full cycle from initial discussion to part production is three to four years in Europe. Having a trusted data resource could save at least six months of groundwork, offering a substantive reduction in design-phase costs, which can represent between ten and twenty per cent of total project cost. A second composite materials developer described materials data as a fundamental enabler without which they would not be able to sell parts or generate revenue, suggesting their technology could be even more effective with better access to materials data.

## Revenue generation and protection

Materials performance data underpins product differentiation, customer value and, in some cases, the ability to sell products at all.

### Protecting revenue through materials performance

A major aerospace business explained that aeroengine materials performance data provides a direct revenue stream from aerospace airframe manufacturers. Materials data is integral to competitive advantage in the aerospace industry. For example, understanding the extent to which thermal barrier coatings enable combustion temperatures above the melting point of the underlying alloy, drives efficiency gains that ultimately determines competitive positioning in the market.

## Safety, regulatory compliance and risk reduction

Trusted data is essential in safety-critical and regulated sectors, where poor information can create major operational, regulatory and reputational risk.

### Speciality chemical company compliance

A specialty chemicals company explained how safety data on powder flammability, which showed a proposed new material to be unsafe, allowed for an alternative to be recommended and prevented a factory from needing a costly ATEX rating upgrade, potentially saving several million pounds.

## Cost reduction and process optimisation

Better materials data can improve throughput, avoid failure events and reduce unnecessary testing, rework and waste.

### Reducing process failure costs

A materials data and IoT business reported that premature resin self-catalysis was costing one customer six figures every two days, with single resin failure events costing well over £100,000 and tank cleaning alone costing upwards of £30,000. This illustrates how better materials data and monitoring can reduce costly process failures and improve operational control.

## Sustainability and the circular economy

Traceability and material knowledge support higher-value recovery, better reuse and stronger environmental performance.

### Unlocking higher-value sustainability and recovery

A major UK recycling business noted that sophisticated recycled aluminium grades command a premium of two to three hundred pounds per tonne, while recycled steel carries a smaller premium of ten to twenty pounds per tonne but applies across millions of tonnes, meaning the aggregate value is substantial. Achieving these premiums depends on being able to characterise and verify the composition of recycled material, making materials data essential to unlocking higher-value recovery from end-of-life assets.

## Supply-chain resilience and market access

Provenance, traceability and auditable manufacturing data are increasingly important for customer confidence, legislation and access to regulated markets.

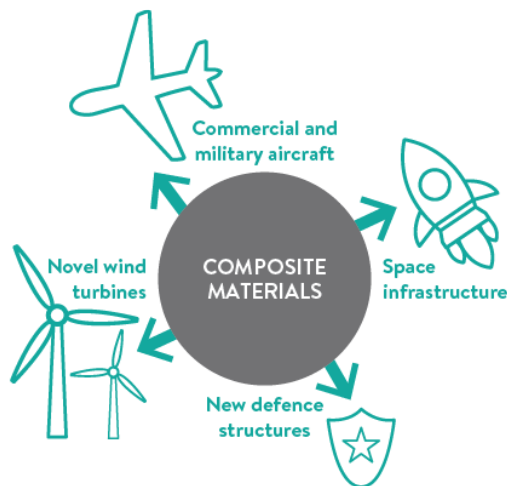
### Traceability as a route to market access

A battery materials interviewee highlighted that battery passports, providing traceability, carbon footprint data and recycling instructions, are becoming commercially important across the wider battery sector. This illustrates how Materials 4.0 capabilities increasingly support access to regulated markets as well as supply-chain resilience.

# Example Use Cases

This series of exemplar use cases demonstrates the benefits of Materials 4.0 and the practicalities of achieving them. They have been developed in collaboration with industry experts and are aligned with the national framework.

## Composite Materials: From trial and error to predictive design



### The challenge

Composite materials are embedded in some of the UK's most strategically important industries. Offshore wind turbines, commercial and military aircraft, defence structures, and emerging space infrastructure all depend on composites that are lighter, stronger and more durable than conventional alternatives. This creates industrial opportunity and scope for civil-defence dual use, where materials knowledge, qualification evidence and manufacturing capability have value across both domains. Yet the processes

by which these materials are designed, manufactured and validated have changed relatively little in decades.

Development still relies heavily on physical prototyping and test campaigns. The links between processing, resulting microstructure, service-life performance, and recycling or re-use are not fully exploited, with limited integration across the materials value chain with a lack of recognised standards. The result is slow development cycles, high costs, and a persistent gap between what materials science can predict, what manufacturers can reliably produce, and how composites are used to maximise useful life.

### Why this matters now

The challenge is sharpening as industries push composites into larger, more complex applications. A wind turbine blade manufacturer scaling to next-generation rotor sizes, or an aerospace supplier qualifying a new structural component, faces the same fundamental problem: understanding how manufacturing decisions affect lifetime performance still requires too many physical trials for the pace and cost the market demands. For example in the wind turbine industry:

## Current constraints

- Charge placement optimisation for pressed composite structures requires extensive physical trialling
- Drapability and fibre orientation prediction depends on experience rather than predictive models
- Thickness variation and lifetime prediction for large structures lacks reliable digital tools
- Data generated across one programme rarely informs the next

## Consequence

- Failures discovered late in development, driving rework and cost
- Slow R&D cycles that cannot keep pace with market and policy demand
- Inconsistent manufacturing quality and difficulty scaling new materials
- Institutional knowledge lost rather than retained and reused

## How Materials 4.0 changes the dial

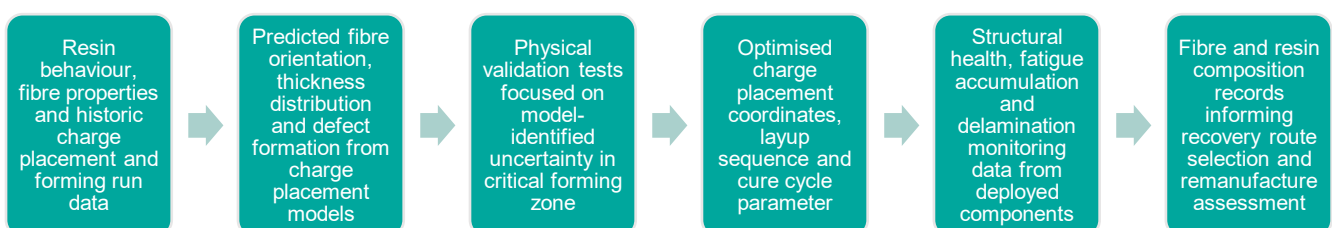
In composites, Materials 4.0 replaces trial and error with predictive, data-driven insight. It does not remove physical testing, but changes its role. By combining forming behaviour, fibre flow and historical process data early in design, models can predict how manufacturing decisions affect structural performance before a prototype is built.

Optimisation tools then identify promising manufacturing configurations, which are validated through a small number of targeted tests. Results are fed back into a shared data environment, improving predictions for future programmes and creating robust, shareable data assets that support collaboration, reuse and competitive advantage. Adoption of these methods is already happening in high value composite manufacturing.

## A federated composite workflow in practice

A manufacturer developing a pressed composite structural part uses Materials 4.0 tools and shared federated datasets to move from repeated physical trialling towards predictive design and targeted validation. As the figure shows, data from design, manufacture, testing, deployment and recovery is linked through a shared environment, giving manufacturing, quality and certification teams a stronger evidence base. Products also gain value when accompanied by robust, shareable data that supports through-life decisions, including recycling and re-use.

### Data flow across the value chain



At each stage, composites data is structured, attributed and returned to the shared environment, creating a continuously improving knowledge base rather than isolated project records.

## What changes compared with today

For researchers and engineers	For decision makers and funders
<ul style="list-style-type: none"> <li>• Fewer prototypes and unnecessary tests</li> <li>• Earlier identification of manufacturing issues</li> <li>• More consistent production and tighter process windows</li> <li>• Faster R&amp;D cycles and better whole-life predictions</li> <li>• A move from experiential practice to evidence-based design</li> <li>• Greater reuse of trusted data between programmes rather than repeated rediscovery</li> </ul>	<ul style="list-style-type: none"> <li>• Clearer cost-performance trade-offs from scenario-based modelling</li> <li>• Stronger, data-supported evidence for certification</li> <li>• Shared infrastructure that benefits multiple programmes and sectors</li> <li>• A more competitive UK position in offshore wind, aerospace, and space</li> <li>• Increased product and supply-chain value through robust, shareable data linked to materials and components</li> <li>• Stronger civil-defence relevance through transferable evidence and capability across domains</li> </ul>

## What is needed to realise this

Realising this at national scale requires shared infrastructure that does not yet exist. Federated data platforms that allow composite materials and process datasets to be shared securely across organisations, validated forming and lifetime models that reflect the diversity of UK industrial practice, and digital integration between design environments and manufacturing equipment are all essential. While other sectors have shown that the UK has the underlying digital capability, composites still needs the governance, standards and support required to use it effectively across the value chain. This matters not only within composites manufacturing, but also where composites interface with coatings, surface treatments, joining systems and non-composite materials in real products and supply chains.

These are not challenges that any single composite manufacturer or research group can resolve alone. They require coordinated investment in shared infrastructure, common data standards, and the skills to work across the boundary between computational modelling and physical manufacturing.

Technical enablers	National and programme levers
<ul style="list-style-type: none"> <li>• Federated data infrastructure and open materials and process datasets</li> <li>• Validated forming and lifetime models</li> <li>• Digital integration with manufacturing tools and equipment</li> <li>• Scalable datasets for composites and alternative fibre systems</li> </ul>	<ul style="list-style-type: none"> <li>• Funding for AI-enabled materials design tools and testbeds</li> <li>• Cross-sector data sharing frameworks and governance</li> <li>• Skills investment in simulation, optimisation, and data practice</li> <li>• Evidence-based certification pathways for data-supported qualification</li> </ul>

## The broader opportunity

The composite materials use case is not a distant aspiration. The building blocks already exist across the UK research and industrial base. The Henry Royce Institute, National Composites Centre, the Catapult network, and a strong university research community provide the foundation. What is needed is the coordination, shared standards and access to the available digital infrastructure to connect them into a coherent national capability. In that model, competitiveness comes not only from better composite products and processes, but also from the ability to generate, retain, share and potentially monetise trusted data assets that create value across programmes, organisations and sectors.

# Nuclear Steels: Lifetime assessment, in-service monitoring and life extension

## The challenge

Nuclear reactor components operate in some of the most demanding conditions of any engineered structure. Pressure vessels, primary circuit pipework, and core structural steels are subject to decades of irradiation, thermal cycling, and mechanical stress in environments where access for inspection is severely constrained and the consequences of material failures are significant.

The full through-life records of nuclear steels have often been poorly maintained, sitting in disconnected systems across multiple owner-operators. Original manufacturing documentation may be incomplete or inaccessible, so links between processing history, irradiation exposure, microstructural change and mechanical performance must often be reconstructed rather than read from a coherent digital record. Where these records are not connected to later inspection and surveillance data, the safety case becomes harder to sustain as assets age. Safety substantiation therefore remains highly manual, reliant on the judgement of a small specialist community, with limited systematic retention of knowledge.

## Emerging pressures

These challenges are now intensifying across multiple fronts, creating new opportunities for action.

## Life extension of existing plant

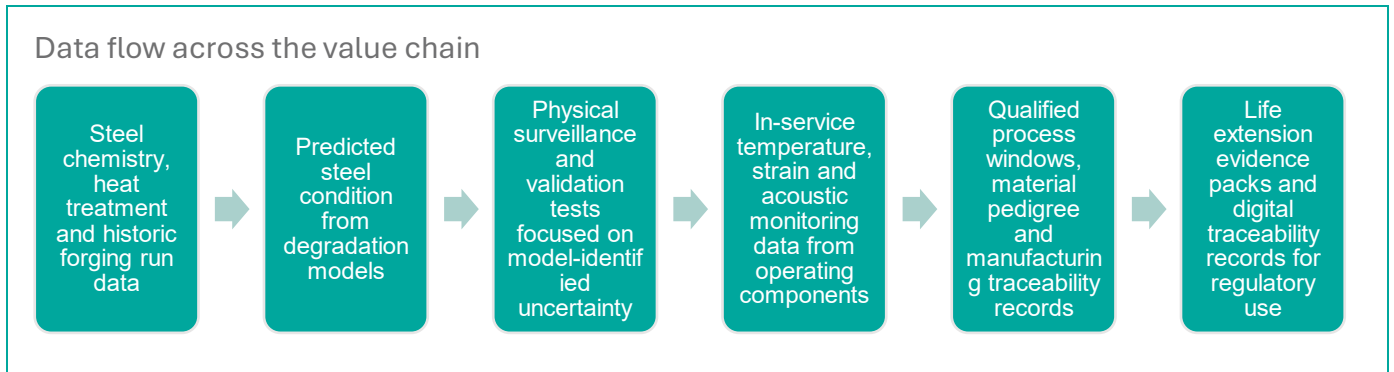
As the existing nuclear fleet ages, life extension decisions depend increasingly on the ability to connect original manufacturing records, irradiation history, surveillance evidence and in-service measurements into a coherent view of component condition. Where those records are incomplete, inaccessible or disconnected, safety substantiation becomes more manual and conservative, leaving operational value unrealised and placing greater burden on a small specialist community. More structured, traceable materials data would support stronger digital safety cases, better targeted follow-on testing and more confident decisions on inspection, maintenance and life extension.

## SMR and AMR deployment and qualification

SMR and AMR programmes are likely to increase demand for nuclear-grade steel components at a scale and pace the existing supply chain has not had to meet for decades. Multiple-unit deployment will also generate far larger volumes of manufacturing and materials data than conventional station builds, creating pressure to capture and reuse evidence efficiently across repeated manufacture. At the same time, qualification remains critical: many SMR vendors are likely to favour established forging and manufacturing routes to reduce risk, while wider SMR/AMR programmes are interested in approaches that could shorten lead times, improve repeatability or reduce waste. Realising those benefits depends on structured process-property datasets and digital capture of manufacturing evidence from the outset.

## Defence nuclear demand

Growing requirements from the defence nuclear sector, including submarine propulsion programmes, place additional demands on material traceability and through-life performance assurance. Security of supply and demonstrable chain of custody from raw material to in-service component are requirements that conventional documentation-based approaches struggle to satisfy at the level of rigour now expected.



## What changes compared with today

For researchers and engineers	For decision makers and funders
<ul style="list-style-type: none"> <li>Structured process-property datasets accelerate assessment of emerging manufacturing routes across programmes</li> <li>Life extension assessments grounded in a traceable material passport history rather than reconstructed from fragments.</li> <li>Materials variability data for probabilistic based design and certification</li> <li>Targeted surveillance and testing focused on genuine uncertainties, reducing cost and access burden</li> </ul>	<ul style="list-style-type: none"> <li>Qualification pathways accelerated by validated datasets for emerging SMR/AMR manufacturing routes</li> <li>Structured, auditable evidence bases that support more efficient safety case review across civil and defence programmes.</li> <li>A sovereign UK capability in nuclear steel supply, grounded in data-assured manufacturing and traceability</li> <li>Steel datasets available as a shared asset</li> </ul>

## What is needed to realise this

The nuclear sector presents data-sharing challenges: long asset lifetimes require governance that survives changes of ownership and operator; security requirements constrain openness, particularly for defence applications; and expertise is concentrated in a few organisations.

Technical enablers	National and programme levels
<ul style="list-style-type: none"> <li>Secure federated data platforms connecting manufacturing,</li> </ul>	<ul style="list-style-type: none"> <li>SMR and defence nuclear programmes specify digital data</li> </ul>

operational and surveillance records across programmes

- Digital capture of manufacturing parameters in standardised forms
- Validated physics-based and machine learning degradation models for irradiation embrittlement and thermal ageing
- Embedded and remote sensing for continuous condition monitoring in access-constrained environments
- Standardised data schemas for nuclear materials records

infrastructure as a supply chain requirement from the outset

- UKRI investment in shared degradation model development, novel forging process datasets, and validation infrastructure
- Regulatory agreement on how digital material records support safety cases through linked manufacturing, surveillance and degradation evidence
- Cross-operator data sharing frameworks for the existing civil fleet, with appropriate security governance for defence data

### The broader opportunity

The UK has a long history of nuclear operation, a deep body of accumulated materials knowledge, and an emerging SMR programme that places it at the forefront of next-generation nuclear development. Connecting that knowledge into a coherent digital environment across life extension, new build and defence applications, and grounding it in the Materials 4.0 framework, would create a national capability that strengthens safety and economics, supports sovereign supply, and positions the UK as a leader in data-driven nuclear materials practice.

# Batteries: From fragmented traceability to circular, data-enabled battery value chains

## The challenge

Batteries are central to the UK's net zero and clean energy transition, underpinning electrified transport, grid flexibility and energy storage. The UK battery strategy<sup>19</sup> explicitly links battery capability to economic prosperity, supply-chain resilience and the transition to a low-carbon energy system, while the UK Critical Minerals Strategy<sup>20</sup> frames security of the raw materials as essential to growth, national resilience and clean energy.

The UK has key strengths especially in battery research and innovation (e.g. through the Faraday Institution<sup>21</sup>, UKBIC<sup>22</sup> and AMBIC<sup>23</sup>) working alongside start-ups and specialist firms. However, the UK faces challenges in delivering a scaled, joined-up industrial capability across the wider sector. Two of the most critical challenges are the following:

- Battery supply chains depend on critical minerals such as lithium, nickel, cobalt, graphite and rare earth elements, where mining, refining and processing are globally concentrated and vulnerable to geopolitical shocks.
- The UK battery value chain remains fragmented with provenance, process history, carbon footprint, state of health and end-of-life data often held in disconnected systems that are difficult to exchange or trust across organisational boundaries. Data is generated at every stage, but it is rarely connected between organisations in a digital thread.

The UK battery strategy and Critical Minerals Strategy both conclude that long-term UK resilience will be dependent on the ability to secure, trace, recover and reuse battery materials more effectively. Future competitiveness will not be determined only by who can manufacture cells at scale, but also by who can manage battery materials, data and recovery most effectively across the full lifecycle, building on the UK's strengths in innovation, industrialisation and specialist capability.

## Why this matters now

These challenges are becoming more urgent because the global battery landscape is changing quickly, and the UK risks being left behind:

- China remains the dominant actor across battery minerals trade, refining and manufacturing, including a leading role in interregional trade in raw battery minerals, battery materials, packs and components.

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<sup>19</sup> [UK battery strategy](#)

<sup>20</sup> [UK Critical Minerals Strategy](#)

<sup>21</sup> The Faraday Institution, [About - The Faraday Institution](#)

<sup>22</sup> UK Battery Industrialisation Centre, [UKBIC](#)

<sup>23</sup> Advanced Materials Battery Industrialisation Centre, [AMBIC](#)

- The United States is using industrial policy and public funding to build domestic capacity in battery materials processing, manufacturing and recycling, explicitly to strengthen energy security and reduce dependence on external supply chains.
- The EU Battery Regulation will require a battery passport covering identity, carbon footprint, due diligence, materials composition, circularity, performance and durability.

This means the UK's window for building distinctive capability is narrowing. Battery competitiveness is now shaped not only by technology performance, but also by traceability, regulatory readiness, supply-chain resilience and the ability to recover more value across the full lifecycle through reuse, repurposing and recycling of critical materials.

### How Materials 4.0 changes the dial

Materials 4.0 helps the UK respond to these challenges by connecting materials, manufacturing, operation and recovery through better data, modelling and digital infrastructure. In practice, that means supporting four things at once:

- Stronger traceability of critical materials.
- Faster and more reliable scale-up from innovation to production.
- Optimisation of in-service life and material degradation.
- Better recovery of value through reuse, repurposing and recycling.

This is aligned with the UK battery strategy's emphasis on innovation, industrialisation and circularity, and with the growing importance of battery passport readiness. For many UK firms, these capabilities will increasingly become necessary. As the EU battery passport comes into force, batteries placed on the EU market will increasingly need to be supported by trusted lifecycle data, making this framework an important reference point for UK battery traceability, circularity and regulatory readiness.

### From fragmented supply chains to traceable, circular materials

Materials 4.0 can strengthen UK resilience by making battery materials easier to trace, govern and recover across the lifecycle. By linking provenance, processing history, carbon footprint and end-of-life information, it supports both battery passport requirements and stronger circular use of critical materials. This helps the UK build advantage in midstream processing, recycling and recovery, rather than relying only on virgin supply or cell manufacturing scale.

### From lab success to scalable industrial capability

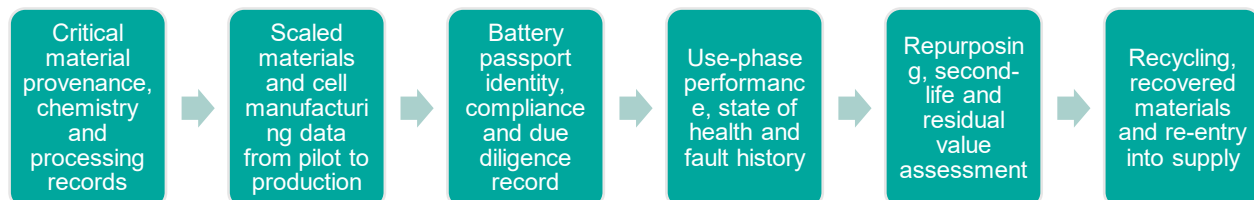
Materials 4.0 can help close the gap between UK innovation strength and wider industrial scale-up. By linking R&D data, pilot-line results, manufacturing quality data and in-service performance, it becomes easier to validate new materials, de-risk scale-up and improve process control. That is relevant to the UK's industrialisation base, including UKBIC and AMBIC, which are intended to help move battery technologies from materials development towards commercial production.

### A federated battery workflow in practice

A battery developer or manufacturer uses Materials 4.0 tools and federated datasets to link battery materials development, manufacturing, operation and recovery through a

shared digital thread. As in the Battery Passport model, data is structured around a unique battery identity and can include materials provenance, carbon footprint, due diligence, composition, performance, state of health and circularity information. Data remains with the organisations best placed to manage it, but can still be discovered, exchanged and updated through agreed standards, identifiers and access rules. This supports battery passport readiness, helps de-risk scale-up from materials innovation to production, and improves decisions on reuse, repurposing and recycling.

#### Data flow across the value chain



At each stage, battery data is structured, attributed and returned to a federated digital environment, creating an evolving lifecycle record rather than isolated project data. This type of operating model will increasingly need to be adopted by UK firms if they are to support battery passport requirements and recover more value from batteries and critical materials across the full lifecycle.

#### What is needed to realise this

Realising this opportunity will require an enabling approach that links battery research, scale-up, manufacture, use and recovery through trusted data and shared standards across the UK battery ecosystem. This would allow evidence to travel with materials and batteries across the lifecycle, helping to de-risk scale-up, understand performance through use, and improve reuse, repurposing and recycling of critical materials, while supporting battery passport readiness where needed.

##### Technical enablers

- Common battery identifiers and metadata to support lifecycle traceability.
- Validated models for battery degradation, process optimisation and second-life assessment.
- FAIR sharing of battery research, pilot and industrial evidence to support scale-up.
- Interoperability standards and interfaces for cross-organisational data exchange, alongside analysis of sector-wide battery data readiness against passport requirements.

##### National and programme levers

- Investment in programmes that connect R&D, pilot and industrialisation activity across the battery ecosystem.
- Support for demonstrators and validation environments that show federated battery data flows in practice.
- Treating battery passport readiness as an industrial capability issue for UK firms supplying into EU markets.
- Sector-wide standards and frameworks to harmonise battery data and traceability.

- Digital and data skills to work in a governed federated environment.
- Support for midstream processing, recycling, reuse and repurposing capability.

### **The broader opportunity**

The UK has a strong battery research base, growing industrialisation infrastructure and a set of specialist capabilities spanning materials innovation, scale-up, modelling and circularity. Key organisations such as the Faraday Institution, Henry Royce Institute, UKBIC and AMBIC provide a base for growth. Connecting those strengths through a Materials 4.0 approach in a more coherent digital environment would help turn fragmented capability into a more durable national proposition aligned with key government strategy areas. This would enable faster scale-up of new battery materials and processes, strengthen traceability and battery passport readiness, and improve reuse and recycling of critical materials. In doing so, it would help the UK compete not only through battery performance, but through trusted data, circularity and industrial resilience, positioning UK firms to capture greater value from the clean energy transition and from battery supply chains serving both domestic and European markets.

# Materials 4.0 Challenges

Beyond the specific digital aspects and sector-specific deployments, there are common challenges to the implementations of Materials 4.0. The materials community each have a role in tackling these challenges in a coordinated and balanced manner.

## Current Materials 4.0 cross-sector challenges

A representative sample of 11 active stakeholders and the National Materials Innovation Strategy steering group for Materials 4.0 were consulted in Phase 1 of the framework's development. This consultation identified a series of cross-sector challenges that were cross-compared with a literature review to produce a set of seven challenges that are barriers to the implementation of Materials 4.0 in the UK.

### Challenge 1: Interoperability and shared semantics<sup>24,25</sup>

**Shared data languages with common property names and definitions are underdeveloped.** Properties of materials, such as microstructure descriptors, processing parameters and derived features, are not encoded consistently. Two datasets may use the “same” property name but have different definitions. Resources and funding are unnecessarily spent on “glue code” that connects different semantic systems together and allows data to interoperate.

### Challenge 2: Data availability, quality, and “FAIR-ness”<sup>26,27</sup>

**Large, longitudinal data sources that adhere to FAIR principles are required for Materials 4.0 but are either scarce or inaccessible.** So-called “dark data” could be unpublished, locked or siloed in an inaccessible format, like PDFs, Laboratory Information Management Systems (LIMS), or spreadsheets. Datasets can lack the metadata needed for meaningful reuse, or not include negative or failed runs, creating biases. Resources are disproportionately spent on data sourcing, curation, cleaning and de-biasing, and there is uncertainty over the value of cleaning existing data versus creating new data.

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<sup>24</sup> Rumble, J.R. Accessing Materials Data: Challenges and Directions in the Digital Era. *Integr Mater Manuf Innov* 6, 172–186 (2017). <https://doi.org/10.1007/s40192-017-0095-2>

<sup>25</sup> Fatima Zivic, Ana Kaplarevic Malisic, Nenad Grujovic, Boban Stojanovic, Milos Ivanovic,

Materials informatics: A review of AI and machine learning tools, platforms, data repositories, and applications to architected porous materials, *Materials Today Communications*, Volume 48, 2025, 113525, ISSN 2352-4928. <https://doi.org/10.1016/j.mtcomm.2025.113525>.

<sup>26</sup> L.Himanen, A.Geurts, A. S.Foster, P.Rinke, Data-Driven Materials Science: Status, Challenges, and Perspectives. *Adv. Sci.* 2019, 6, 1900808. <https://doi.org/10.1002/advs.201900808>

<sup>27</sup> LC Brinson, LM Bartolo, B Blaiszik, D Elbert, I Foster, A Strachan, PW Voorhees, Community Action on FAIR Data will Fuel a Revolution in Materials Research. <https://arxiv.org/pdf/2204.02881>

### Challenge 3: IP, cybersecurity, and governance across multi-stakeholder ecosystems<sup>28,29</sup>

**Details of material formulations and processes are intellectual property (IP) that grants the holder a competitive edge.** Sharing of this data through the supply chain and across collaborators presents a risk. Machine Learning models and cross-organisation interfaces are a source of potential leaks or vulnerabilities. Industry won't share this high-value property and process data without governance procedures, access controls, and auditability.

### Challenge 4: Model credibility in physical applications vs “black box” applications<sup>30,31,32</sup>

**Models used and proven in research scenarios are too complex to translate into industry use.** The models need to be recalibrated to account for the multiscale conditions of their use in industrial settings, and not in silico (i.e., entirely digital). The models are not designed for physical applications and particularly the certainty needed for expensive and safety-critical applications. Digital twins require continuous data flows, calibration, and provenance across processes.

### Challenge 5: Reliable integration of automated processes<sup>33,34,35</sup>

**Automated Materials 4.0 processes (automated labs and unsupervised learning algorithms) work in defined, experimental settings, but don't work at scale.** When used in lab settings, they are run on specific exemption, rather than the standardised and repeatable processes required in manufacturing settings. Machines and processes that successfully automate at the microgram scale can't be scaled to larger quantities.

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<sup>28</sup> Wong, Hoo Meng & Mohamad, Siti Farah Norbaini. (2024). The Data Governance: A Comprehensive Literature Review from Professional Viewpoints. 10.13140/RG.2.2.16052.87683.

<sup>29</sup> Claravine. Data Governance Frameworks: The Cornerstone of Data-Driven Enterprises. (2023). <https://www.claravine.com/resources/data-governance-framework/>

<sup>30</sup> Kalidindi SR, Buzzy M, Boyce BL and Dingreville R (2022), Digital Twins for Materials. *Front. Mater.* 9:818535. doi: 10.3389/fmats.2022.818535

<sup>31</sup> Deagen, M.E., Brinson, L.C., Vaia, R.A. et al. The materials tetrahedron has a “digital twin”. *MRS Bulletin* 47, 379–388 (2022). <https://doi.org/10.1557/s43577-021-00214-0>

<sup>32</sup> Daniel Cogswell and Chaitanya Paramatmuni and Lucia Scotti and James Moffat, Guidance for Materials 4.0 to interact with a digital twin, *Data-Centric Engineering*, volume (3), (2022), <https://api.semanticscholar.org/CorpusID:249281905>

<sup>33</sup> Gary Tom, Stefan P. Schmid, Sterling G. Baird, Yang Cao, Kouros Darvish, Han Hao, Stanley Lo, Sergio Pablo-García, Ella M. Rajaonson, Marta Skreta, Naruki Yoshikawa, Samantha Corapi, Gun Deniz Akkoc, Felix Strieth-Kalthoff, Martin Seifrid, and Alán Aspuru-Guzik. *Chemical Reviews* 2024 124 (16), 9633-9732. DOI: 10.1021/acs.chemrev.4c00055

<sup>34</sup> Alexander V. Tobias, Adam Wahab; Autonomous ‘self-driving’ laboratories: a review of technology and policy implications. *R Soc Open Sci.* 1 July 2025; 12 (7): 250646. <https://doi.org/10.1098/rsos.250646>

<sup>35</sup> Szymanski, N.J., Rendy, B., Fei, Y. et al. An autonomous laboratory for the accelerated synthesis of inorganic materials. *Nature* 624, 86–91 (2023). <https://doi.org/10.1038/s41586-023-06734-w>

## Challenge 6: Qualification, standards, and regulatory acceptance (especially for safety-critical materials)<sup>36</sup>

**Sectors with strict safety cases have high standards in qualifying models.** To deploy new materials models in, for example, aerospace, nuclear, medical, or infrastructure contexts, they will require intensive qualifications. These processes may negate the time saved in their deployment. Regulated adoption demands auditable datasets, documented uncertainty, and defensible validation – often at a higher rigour than typical ML papers. In these sectors, product lifecycles are long, and there is a culture of labour-intensity and diligence, holding back innovation.

## Challenge 7: Incentives (including economic), culture, skills, and organisational change<sup>37</sup>

**Materials 4.0 requires sustained data stewardship and software-like practices (versioning, documentation, monitoring), which many materials organisations are not set up to reward.** New and hybrid skills that blend materials science with automation, statistics, software, and computer science are needed. Access to computing power is a barrier to adoption. Data governance is seen as extra work, without economic reward, and pilot projects do not get maintained or scaled. Funding is intermittent and scattered across disciplines and sectors.

## Challenge Prioritisation

An online survey was run to test the challenges with the UK materials community and understand the priorities, barriers and potential mitigation actions.

A key outcome of the survey was the prioritisation of the cross-sector challenges, to understand the UK community's perceived barriers. Overall, the most critical challenge was Challenge 2: Data availability, quality and “FAIR-ness”, with 26% of respondents indicating it was the highest priority challenge.

Challenge	Rank
<b>C2. Data availability, quality, and “FAIR-ness”</b>	1
<b>C7. Incentives (including economic), culture, skills, and organisational change</b>	2
<b>C1. Interoperability and shared semantics</b>	3
<b>C3. IP, cybersecurity, and governance across multi-stakeholder ecosystems</b>	4

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<sup>36</sup> Cogswell D, Paramatmuni C, Scotti L, Moffat J. Guidance for Materials 4.0 to interact with a digital twin. *Data-Centric Engineering*. 2022;3:e21. doi:10.1017/dce.2022.23

<sup>37</sup> L. Hung, J. A. Yager, D. Monteverde, D. Baiocchi, H.-K. Kwon, S. Sun and S. Suram, Autonomous laboratories for accelerated materials discovery: a community survey and practical insights. *Digital Discovery*, 2024, 3, 1273—1279. <https://doi.org/10.1039/d4dd00059e>

<b>C4. Model credibility in physical applications vs “black box” applications</b>	5
<b>C6. Qualification, standards, and regulatory acceptance (especially for safety-critical materials)</b>	6
<b>C5. Reliable integration of automated processes</b>	7

The respondents confirmed that all of the challenge types impact the full materials value chain, with scale-up and material production being the stage where the challenges to Materials 4.0 implementation are strongest.

The survey asked respondents to suggest actions to overcome these challenge and necessary enablers for these actions. The highest priority actions to address these challenges were turned into implementation roadmaps by the workshop attendees (provided in Appendix 3) and these in turn informed the four priority action plans from this framework.

# Priority Action Plans

**The UK materials innovation ecosystem has identified four key priorities for action to overcome pervasive barriers to the adoption of Materials 4.0.**

These are areas where coordinated national activities could have the greatest impact, capturing the opportunity presented by Materials 4.0 to bolster the UK's impactful, global materials innovation capabilities.

## Priority 1: Availability of High-Quality Data

**Valuable materials data is often hard to find, inaccessible, poorly described, difficult to exchange between organisations, or locked in legacy systems.**

To address this, organisations across the materials community need to be empowered to take ownership of their own data and to federate it in ways that support reuse, collaboration and lifecycle connectivity. The priority is therefore to provide the capabilities, standards and enabling functions that allow organisations to work to a clearer and more consistent baseline, while retaining the flexibility needed for different materials contexts, applications and lifecycle requirements.

### Action

Support organisations to generate, manage and share materials data in ways that are consistent, proportionate and reusable, while recognising that different materials, processes and use cases require different levels of structure and detail.

### Activities

- Define a minimum national baseline for materials metadata, quality criteria, lifecycle information and reporting rules, without imposing one fixed format for all use cases. Use publicly funded research and pathfinder activities to drive adoption of this baseline.
- Produce sector- and use-case-specific guidance so organisations can apply common principles proportionately in different materials contexts.
- Support discovery, recovery and improvement of legacy and dark data where there is high reuse or strategic value.
- Invest in tools, stewardship and practical support that help materials focussed organisations adopt FAIR data practices within existing workflows.
- Fund data generation exemplar programmes and require better data practice in publicly funded programmes such that improved approaches are demonstrated and become normalised over time.

## Priority 2: Incentivising Uptake

**Investment in Materials 4.0 activity is already taking place across the UK, but capability remains uneven and adoption is still at an early stage in many parts of the materials community.**

Public funding can play an important enabling role in encouraging activity, supporting demonstrators, building skills and helping emerging approaches move towards wider industrial use. Where this is coordinated at sector level, it can also help establish shared capabilities and reduce future barriers to entry. The priority is therefore to back the incentives, demonstrators and capability-building measures that help organisations adopt Materials 4.0 in practice.

### Action

Use public support, incentives and practical delivery mechanisms to help organisations adopt Materials 4.0 approaches in operational settings, building skills and overcoming cultural differences, while coordinating effort at sector level where this can reduce future barriers to entry.

### Activities

- Introduce targeted incentives, adoption support and challenge funding for organisations seeking to improve their Materials 4.0 capability.
- Use public co-funding to support demonstrators, pilots and pathfinder activities that reduce the risk of early adoption and demonstrate the value.
- Continue to provide the infrastructure, compute access and tools for scalable digital working in pre-competitive environments.
- Back cross-sector research consortium or demonstrators to build best practice and create communities of practice.
- Invest in digital skills and workforce development linked to materials data, modelling, digital tools and deployment.

## Priority 3: Data Interoperability

**Even where materials data exists, it is often difficult to combine, exchange or reuse because definitions, ontologies, formats and software tools are inconsistent.**

Interoperability and shared semantics have been identified as one of the most important cross-sector barriers to Materials 4.0 adoption, with the associated cost of fragmented workflows, bespoke integration and disconnected systems. Organisations need the trusted governance, shared data language and connectivity needed for federated data exchange allowing organisations to connect data, models and workflows more effectively across research, industry and the wider materials lifecycle.

### Action

Enable materials data, software tools and digital workflows to work together across organisational and lifecycle boundaries through shared semantics, interoperable standards and federated approaches to connectivity.

## Activities

- Create a national governance mechanism to maintain semantic assets (materials ontologies, vocabularies and data schemas), with industry participation and standards bodies and international linkages, so that shared semantic assets are curated, aligned and sustained over time.
- Ensure that semantic assets are aligned with international standards.
- Set minimum interoperability expectations for different organisation types and for publicly funded tools, platforms and data environments, including open APIs, shared schemas and machine-readable formats, so that outputs can move more easily from research into industrial use.
- Fund research into AI-enabled semantic quality assurance and automated data migration.
- Build skills in data engineering, ontology development, materials semantics, and coding.
- Support national testbeds and demonstrators that link discovery, manufacturing, qualification and recycling workflows, so that interoperability can be tested and validated in real cross-lifecycle settings.
- Work with commercial vendors and system integrators to ensure UK-funded tools can import and export using shared data languages and interoperable formats, reducing dependence on proprietary or isolated workflows.
- Prioritise interoperability and federated data approaches in strategically important sectors while aligning with key international partners and emerging global standards where this supports resilience, trade and collaboration.

## Priority 4: Security and Governance

**Supply chain actors are protective of certain materials data that they hold. Formulations and processing histories are protectable IPR, and they do not want to share this data in systems that could expose it to competitors.**

The security of data sharing was a persistent concern of the stakeholders engaged in this process. It is a common current working practice to strictly protect materials data where it could offer a competitive advantage, particularly in emerging sectors where a material's formulation or processing could provide it with the performance benefits needed to unlock a new market. Sharing this data for Materials 4.0 processes needs to be secure and traceable, with the correct governance in place to protect the data's owner.

### Action

Create the enabling processes and secure collaboration environments needed for supply chain actors to confidently share their valuable materials data with partners.

### Activities

- Create a trusted research environment or secure collaboration environment as part of a Materials 4.0 demonstrator.

- Identify critical IP with industry and develop a categorisation framework on security levels that can inform metadata semantics.
- Engage with suppliers of similar high-value data industries (particularly pharmaceuticals and finance) to introduce their secure data tools to materials innovation.
- Use established data sharing tools (cloud storage and APIs) to benefit from flexible access controls, authentication and tiered permissions.
- Identify a non-critical pilot or use case for secure data sharing and test a governance process that demonstrates protection of materials data IP in a full supply chain.
- Promote federated approaches to data access and workflow integration, allowing organisations to retain appropriate control of local data while connecting it through shared identifiers, metadata, interfaces and governance mechanisms.
- Translate skills and research capabilities in cyber security, IP and trade secrets into the materials ecosystem.
- Publicly fund cybersecurity experts to research this barrier and transfer knowledge.

# Next Steps

**Materials 4.0 is a strategic capability for the UK, central to productivity, industrial resilience, and scientific leadership. It is critical to realising the national materials innovation strategy and maintaining the UK's leadership in the global materials sector.**

This national framework defines Materials 4.0 across four component areas: data attributes, data infrastructure, algorithms and models, and digital tools and techniques. All areas have attracted investment but need cross-sector focus to develop into valuable, integrated functions.

The UK has the foundations to lead, but requires decisive action across four priorities:

1. Availability of high-quality data
2. Incentivising uptake
3. Data interoperability
4. Security and governance

Suggested actions and activities for addressing these priorities are provided, having been developed in collaboration with the materials community.

Acting on these priorities now will ensure that the Materials 4.0 national framework delivers across the entire innovation supply chain, from fundamental research to industrial deployment and circular recovery, strengthening national competitiveness for the decades ahead.

# Appendices

## Appendix 1: Existing ontologies and international comparisons

### Existing material ontologies and standards

#### Platform Material Digital Ontology (PMDco)

The Platform Material Digital Core Ontology is a domain-specific mid-level semantic framework for materials science and engineering (MSE)<sup>38</sup>. The scope of PMDco follows the fundamental MSE paradigm of processing, structure, and properties, encompassing three core domains. First, processes, covering the representation of MSE-related process chains such as materials manufacturing, characterization, and simulation. Second, structure/state, describing substances and engineered materials, including their composition and multiscale structural features. Third, properties, specifying material properties and qualities and capturing processing–structure–properties dependencies. In addition, PMDco provides general entities required to represent foundational MSE topics (e.g., thermodynamics), as well as cross-disciplinary semantic concepts such as devices, roles, functions, and plans<sup>39</sup>.

#### NFDI MatWerk Ontology (MWO)

The NFDI MatWerk Ontology is a mid-level ontology developed within the German NFDI-MatWerk consortium to support research data management in materials science and engineering. It provides a structured semantic framework for standardising the description of research data, linking distributed datasets, tools, projects, and researchers, and improving interoperability and FAIRness across the MSE domain. Its scope covers consortium structures, digital research resources (such as datasets, software, workflows, and metadata schemas), services and collaborations, and MSE-related instruments and materials<sup>40</sup>.

#### Metadata4Ing

Metadata4Ing is an ontology developed within the NFDI4Ing consortium to provide a semantic framework for the structured description of research data in the engineering sciences and related disciplines. It enables comprehensive representation of the entire data-generation process, including experiments, observations, and simulations, covering the object of investigation, sample preparation and data manipulation

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<sup>38</sup> Bayerlein, B., Schilling, M., Birkholz, H., Jung, M., Waitelonis, J., Mädler, L. and Sack, H., 2024. *PMD Core Ontology: Achieving semantic interoperability in materials science*. *Materials & Design*, 237, 112603. <https://doi.org/10.1016/j.matdes.2023.112603>

<sup>39</sup> MaterialDigital, *core-ontology*, GitHub repository, 2025, <https://github.com/materialdigital/core-ontology>

<sup>40</sup> Beygi Nasrabadi, H., Norouzi, E., Hubaiev, K., Waitelonis, J. and Sack, H., 2025. *NFDI MatWerk Ontology (MWO): A BFO-compliant ontology for research data management in materials science and engineering*. *Advanced Engineering Materials*, e202502331. <https://doi.org/10.1002/adem.202502331>

procedures, associated tools and methods, resulting data files, and the roles of individuals and institutions involved<sup>41</sup>.

### **EMMO (Elementary Multiperspective Material Ontology)**

Focuses on providing a standard representational framework for materials modelling and characterisation. Developed by the European Materials Modelling Council (EMMC), its contributors include researchers from various European institutions. A key development choice was using a "bottom-up" approach, starting from fundamental physical concepts like elementary particles and wave-particle dualism rather than abstract top-level philosophy. This ensures the ontology remains grounded in the perspective of applied physics and materials science, facilitating easier adoption by scientists with limited philosophical backgrounds.

### **MAMBO (Materials and Molecules Basic Ontology)**

Lightweight ontology targeting the intersection of the molecular scale and higher-scale domains, such as nanomaterials and molecular aggregates. It was developed by the DAIMON Lab (CNR, Italy) and the University of Bologna. Development followed a hybrid top-down and bottom-up strategy, utilising domain expert interviews to define competency questions. A core choice was adopting Problem-Solving Methods (PSM) to link knowledge representation directly to operational tasks, ensuring the ontology remains modular and focused on practical research-oriented activities.

### **MDS-Onto (Materials Data Science Ontology)**

Low-level framework unifying knowledge in Materials and Applied Data Science. Led by Case Western Reserve University, contributors include various U.S. Department of Energy national laboratories. The framework establishes a semantic bridge to the Basic Formal Ontology (BFO), often using PMDCo as an intermediary. Key development choices include a modular, automated approach and the creation of bilingual (R/Python) packages like FAIRmaterials and FAIRLinked to streamline the generation of FAIR-compliant datasets.

### **MDO (Materials Design Ontology)**

Focuses on enabling semantic queries and integrated data retrieval across multiple materials databases. It was developed primarily by researchers at Linköping University (Sweden). The ontology is structured around core concepts of Structure, Provenance, and Property to unify experimental and computational results. A central design choice was making the ontology modular, allowing it to handle diverse data from databases like NOMAD or OPTIMADE through specific mappings. This structure supports MDO-enabled query expansion and mediation.

### **GEMD (Graphical Expression of Materials Data)**

Open-source format designed to link materials, production processes, and characterisation measurements. It was initially developed by Citrine Informatics in the United States. The ontology's scope allows for backwards traversal from a measurement

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<sup>41</sup> Arndt, S., Farnbacher, B., Fuhrmans, M., Hachinger, S., Hickmann, J., Hoppe, N., Horsch, M.T., Iglezakis, D., Karmacharya, A., Lanza, G., Leimer, S., Munke, J., Terzijska, D., Theissen-Lipp, J., Wiljes, C. and Windeck, J., 2023. *Metadata4Ing: An ontology for describing the generation of research data within a scientific activity* (Version 1.2.1). Zenodo. <https://doi.org/10.5281/zenodo.10022363>

to the specific material and process that produced it. A significant design choice was making a "first-class distinction" between intent (Spec) and realisation (Run), where a single intent can result in multiple realisations. This choice matures concepts previously established in the Physical Information File (PIF) format.

### Allotrope Taxonomies and Ontologies

Part of a framework designed for the standardisation of analytical data across the laboratory lifecycle. Developed by the Allotrope Foundation, a consortium of member companies and partners, it covers domains such as material, equipment, process, and result. Key choices include the use of HDF5 for binary data storage and RDF for metadata. Furthermore, it employs SHACL (Shapes Constraint Language) to provide a syntactic framework that allows computer systems to automatically verify data structures.

### ISO 10303

The ISO 10303 introduces a series of standards for computer-interpretable representations and exchange of product data across the whole product lifecycle. This ISO standard encompasses information related to product design, validation, testing and measurement, among other relevant contextual information.

### Corresponding high-level classes

Ontology, standards and models	High-level Classes
<b>Materials Data Science Ontology (MDS-Onto)</b>	Department (Abteilung), Algorithm, Picture (Bild), Width (Breite), Calibration Document, Computer node (Computerknoten), Data Acquisition Rate, Description, Distance, Force, Identifier, Labor, Length, Location, ManufacturingProcess, MaterialDesignation, Material property (Materialeigenschaft), Measuring Process, MeasuringDevice, Medium, Metadata (Metadaten), NodeSeries, Furnace (Ofen), Optical, PrimaryData, Probe, Project Identifier, Provided Identifier, Process (Prozess), Process node (Prozessknoten), Sequence Number, SpecimenName, Thickness, Value object (Wertobjekt), WorkingRange, Time
<b>Platform Material Digital Ontology (PMDco)</b>	Activity, Agent, Chemical Entity, Digital Material Identifier, Entity, Fragment Selector, Influence, InstantaneousEvent, Location, Role, Unit
<b>Materials Design Ontology (MDO)</b>	Agent, Angle Triple, Atom, Axis Vectors, Basis, Calculation, Composition, Computational Method, Computational Method Parameter, Coordinate Vector, Exchange Correlation Energy Functional, Lattice, Length Triple, Material, Occupancy, Point Group, Quantity, QuantityKind, QuantityValue, Site, Space Group, Species, Structure, Unit
<b>NFDI MatWerk</b>	Chemical element, Contact point, CreativeWork, Intangible, Large-scale facility, licence, Material, Material, Material, Material condition,

<b>Ontology (mwo)</b>	Material Designation, Material property, Material type, Materialeigenschaft, Media Type, Method, object type, Organised event, Organization, organization, Person, person, place, Product, project, Project, Property, Property, Research group, resource, role, Science, Scientific Instrument Manufacturer, semantic expressivity, service type, software interface, technological means, Technology
<b>Materials And Molecules Basic Ontology (MAMBO)</b>	Algorithm, ComputationalMethod, Coordinates, Experiment, ExperimentalMethod, ExternalCoupling, Integrator, InteractionPotential, LatticeParameter, Material, MaterialProperty, Orientation, PotentialComponent, Simulation, SimulationEnsemble, StructuralEntity, Structure, TopologicalEntities
<b>European Materials Modelling Ontology (EMMO)</b>	Ampere, Atto, BaseQuantity, BaseUnit, Becquerel, Candela, Centi, Collection, Conventional, ConventionalQuantitativeProperty, Coulomb, Deci, DegreeCelsius, Dekka, DerivedQuantity, DerivedUnit, Dispersion, ElectricCurrent, EMMO, Engineered, Exa, ExactConstant, Existent, Farad, Femto, Giga, Gray, Hecto, Henry, Hertz, Icon, Index, IonAtom, Item, Joule, Katal, Kelvin, Kilo, Kilogram, Length, Lumen, LuminousIntensity, Lux, Mass, Massive, Massless, MeasuredConstant, MeasuredQuantitativeProperty, Mega, Metre, Micro, Milli, Model, ModelledQuantitativeProperty, Mole, MultipleUnit, Nano, NeutralAtom, Neutron, Newton, NonPrefixedUnit, ObjectiveProperty, Ohm, OrdinalQuantity, Pascal, Peta, Physical, Pico, PrefixedUnit, Proton, Second, SI CoherentUnit, Siemens, Sievert, SI Non Coherent DerivedUnit, SI Non CoherentUnit, SI Unit Symbol, State, SubjectiveProperty, SubMultipleUnit, Tera, Tesla, ThermodynamicTemperature, Time, Void, Volt, Watt, Weber, Yocto, Yotta, Zepto, Zetta
<b>Metadata4ling</b>	agent, assignment, association, bibliographic record, boolean variable, configuration, dataset, dataset series, distribution, Field, file object, file set, Group, has uncertainty declaration, method, numerical assignment, numerical variable, obsolete coverage interval, obsolete expanded uncertainty, obsolete real, obsolete uncertainty declaration, organization, person, processing step, project, property, quantity kind, quantity value, record set, research project, role, software agent, text variable, tool, value, variable, variable set
<b>ISO 10303:235</b>	Activity, Administration, Approval, Condition, Document management, Effectivity, External reference, Geometry, Geometric tolerance, Location, Measure, Person organisation, Product, Properties, Requirement, Resource, State, Substance, Tolerance datum
<b>Graphical Expression of Materials Data (GEMD)</b>	Material object, Measurement object, Process object, Ingredient object.

<b>Allotrope Framework</b>	Material, Equipment, Process, Result, Object Property, Data Type Property
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## International case study: Germany’s approach to developing ontologies for materials

### Strategy and macro-level governance structure

Germany has a thriving environment for ontologies development for materials science and engineering. The scope of this case study covers over 40 ontology development initiatives in Germany. Across these initiatives, the long-term objective is the development of interoperable materials knowledge ecosystems, within which ontologies function as enabling tools for making data more findable and searchable across institutional and disciplinary boundaries.

In Germany, semantic infrastructure is increasingly treated as a national strategic capability. Public investment is channelled through structured consortia with clearly defined mandates, reflecting the view that sustainable semantic infrastructure requires coordinated national support comparable to that provided for major research facilities.

The initiatives identified in this study can be grouped into three broad streams of ontology development work:

- **Stream 1:** National Research Digital infrastructure (NFDI) funded by German Research Foundation (DFG)
- **Stream 2:** Platform MaterialDigital initiative funded by the Federal Ministry of Education and Research (BMBF)
- **Stream 3:** Independent ontology development work funded by EU grant and other independent institutes

The three streams illustrate how different areas of activity collectively support the development of ontology initiatives in Germany. Stream 1 focuses on research data management across academic disciplines, while Stream 2 advances the digital transformation of materials science and engineering, together with its associated industrial value chains. In addition to these coordinated initiatives, German universities and research organisations also undertake independent ontology development efforts, as summarised under Stream 3.

*A comparison between the three streams of work in terms of funding body, stakeholder type and coverage across the value chain is Table 5 shown in the table below. Table 5: Comparison of ontology development work streams in Germany by funding body, stakeholder type and coverage across materials value chain.*

Overview of German ontology-related initiatives relevant to materials science						
		Stream 1			Stream 2	Stream 3
		NFDI-MatWork	NFDI4I ng	FAIRmat	Platform MaterialDigital	Independent initiatives
Primary funding body	German Research Foundation (DFG)	●	●	●		

	German Federal Ministry of Education and Research (BMBF)				●	
	EU grant funding					●
	Other independent funding (e.g. institute-based)					●
<b>Stakeholder types</b>	National	●	●	●	●	●
	International			●		●
	Academia	●	●	●	●	●
	Industry				●	●
<b>Ontologies coverage across the materials value chain</b>	Raw material extraction				●	
	Material & process discovery and design	●	●	●	●	●
	Synthesis & characterisation	●	●	●	●	●
	Product development				●	●
	Product manufacturing				●	●
	Testing / inspection / certification	●			●	●
	In-service (operation & maintenance)				●	

	Circularity 5Rs				●	
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Source: summarised by IfM Engage

### **Stream 1: National Research Data Infrastructure (NFDI) funded by German Research Foundation (DFG)**

Many initiatives are embedded within the National Research Data Infrastructure (NFDI), which was established in 2020 and is funded by German Research Foundation (DFG). NFDI currently comprises 26 discipline-specific consortia and one cross-consortia body (Base4NFDI). Each consortium is responsible for developing domain-specific research data infrastructures tailored to its respective scientific community.

Within the materials and engineering domains, several NFDI consortia are particularly relevant to ontology development:

- NFDI-MatWerk: Materials Science and Materials Engineering
- NFDI4ING: Engineering Sciences
- FAIRmat: Condensed-Matter Physics and the Chemical Physics of Solids

While all operate within the German NFDI framework, they differ in disciplinary scope and semantic orientation.

**NFDI-MatWerk consortium** places a strong emphasis on ontology engineering and the development of a structured semantic backbone for materials science and engineering.

The consortium aims to build a FAIR-compliant (Findable, Accessible, Interoperable, and Reusable) community-driven materials research data infrastructure by developing interoperable ontologies, enabling access to materials data and metadata, and providing shared tools, workflows, and user-centric guidance that connect heterogeneous data, models, and analysis methods across materials science<sup>42</sup>.

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<sup>42</sup> German National Research Data Infrastructure (NFDI), *NFDI-MatWerk: National Research Data Infrastructure for Materials Science and Engineering* [online]. Available at: <https://www.nfdi.de/nfdi-matwerk/?lang=en>

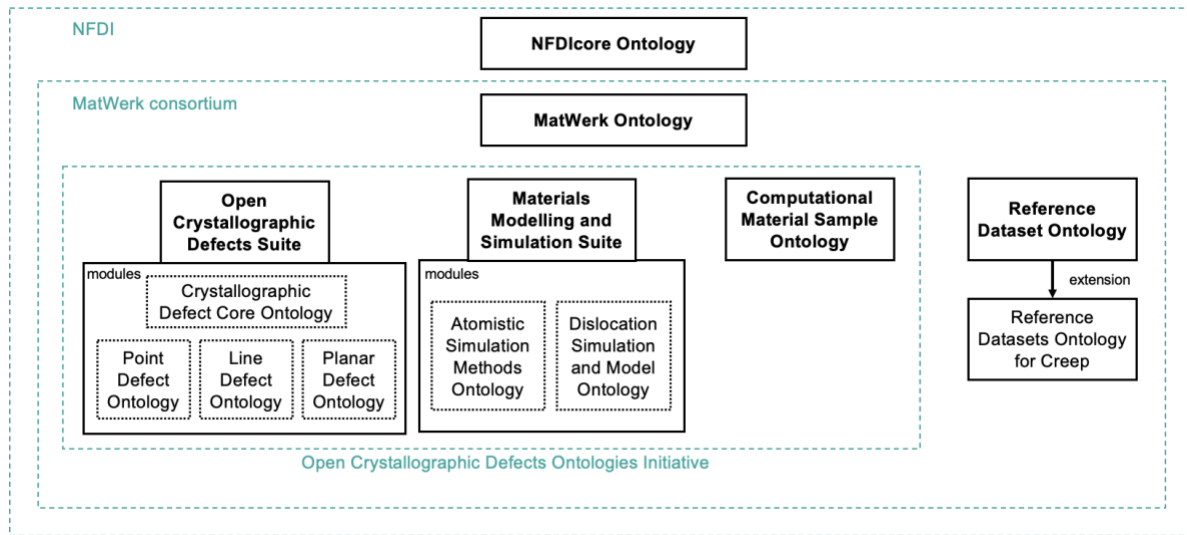


Figure 9: An overview of ontology initiatives within the NFDI-MatWerk consortium. Source: summarised by IfM Engage

**NFDI4Ing consortium** places a strong emphasis on the coordination of research data management practices and the harmonisation of metadata across engineering disciplines.

The consortium aims to establish a sustainable, community-driven research data infrastructure for engineering sciences by developing shared standards, metadata models, and services that support the management, integration, and reuse of heterogeneous engineering research data across diverse workflows and disciplinary contexts.

The NFDI4Ing consortium operates through a structured work programme organised into domain-oriented archetypes and cross-cutting task areas. Archetypes represent characteristic engineering research workflows and data challenges, providing a needs-driven framework for developing research data management solutions. Complementing these are transversal task areas addressing infrastructure services, metadata, and community coordination.

A key initiative within the consortium is the Special Interest Group (SIG) Metadata & Ontologies, which acts as a coordination and development forum for metadata modelling and semantic technologies. Through structured exchange across archetypes, community clusters, and infrastructure services, the SIG ensures that metadata solutions respond directly to real research data management challenges<sup>43</sup>.

A key contribution of SIG is realised through its subgroup Metadata4Ing, which develops a metadata and ontology model tailored to engineering research infrastructures<sup>44</sup>.

**FAIRmat consortium** is dedicated to developing a FAIR research data infrastructure for materials and condensed-matter science. Its objective is to enable researchers to make

<sup>43</sup> NFDI4Ing, *Consortium* [online]. Available at: [https://nfdi4ing.de/home/25\\_aboutus/25\\_consortium/](https://nfdi4ing.de/home/25_aboutus/25_consortium/)

<sup>44</sup> NFDI4Ing, *Metadata & Ontologies* [online]. Available at: <https://nfdi4ing.de/metadata-ontologies/>

data FAIR-compliant across experimental, computational, and theoretical materials research<sup>45</sup>.

FAIRmat collaborates with international initiatives such as the Research Data Alliance (RDA), the European Open Science Cloud (EOSC), and GO FAIR, and maintains partnerships with international research organisations<sup>46</sup>.

The consortium builds upon the NOMAD Laboratory infrastructure and extends it to additional materials science domains. It is organised into thematic areas covering synthesis, experiment, computation, infrastructure development, and coordination. Ontology and metadata development within FAIRmat are embedded directly within its infrastructure architecture.

Semantic modelling is coordinated under Area D (Infrastructure), Task D1: Metadata, Ontologies, and Workflows, led by the Max Planck Computing and Data Facility (MPCDF) and the Karlsruhe Institute of Technology (KIT). Rather than establishing a standalone layered ontology stack, FAIRmat integrates semantic modelling directly with repository architecture and workflow design<sup>47</sup>.

A key ontology developed within FAIRmat is the Provenance Information in Materials Science (PRIMA) ontology, which provides a semantic framework for representing provenance information across experimental and computational workflows in materials research.

### ***Stream 2: Platform MaterialDigital initiative funded by the Federal Ministry of Education and Research (BMBF)***

The Federal Ministry of Education and Research (BMBF) funds the Platform MaterialDigital initiative. Unlike the National Research Data Infrastructure (NFDI), which focuses primarily on research data management across academic disciplines, Platform MaterialDigital aims to advance the digital transformation of materials science and engineering and its associated industrial value chains.

Launched in 2019, the initiative seeks to improve interoperability and reuse of materials data across institutional and organisational boundaries by developing shared semantic foundations, technical standards, and decentralised digital infrastructures for materials data.

A key component of this effort is the development of domain ontologies and semantic models that enable machine-readable descriptions of materials, processes, and workflows across the materials life cycle. The initiative also acts as a central contact point for stakeholders seeking to engage with digitalisation activities, contributing to a shared roadmap that aligns national strategy with international developments.

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<sup>45</sup> FAIRmat, *Tutorials* [online]. Available at: <https://www.fairmat-nfdi.eu/fairmat/outreach-fairmat/tutorials-fairmat>

<sup>46</sup> FAIRmat, *Consortium FAIRmat* [online]. Available at: <https://www.fairmat-nfdi.eu/fairmat/about-fairmat/consortium-fairmat>

<sup>47</sup> FAIRmat, *Area D: FAIRmat* [online]. Available at: <https://www.fairmat-nfdi.eu/fairmat/areas-fairmat/area-d-fairmat>

Platform MaterialDigital platform brings together several leading German research organisations, including Fraunhofer IWM, Karlsruhe Institute of Technology (KIT), IWT Bremen (Leibniz Institute for Materials Engineering), a Max Planck Institute, BAM (Bundesanstalt für Materialforschung und -prüfung), Fraunhofer AISEC, and FIZ Karlsruhe<sup>48</sup>.

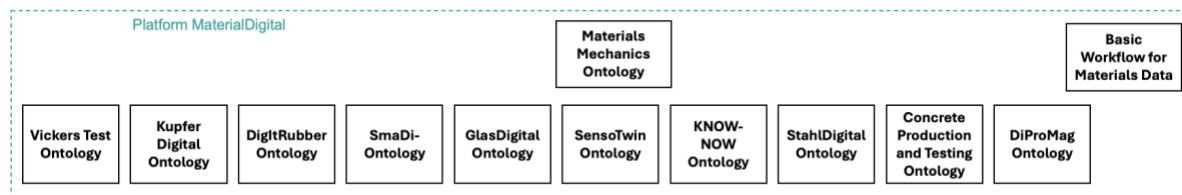


Figure 10: An overview of ontology initiatives in Platform MaterialDigital

### Stream 3: Independent ontology development work funded by EU grant and other independent institutes

In addition to the previously mentioned coordinated initiatives, German universities and research organisations also undertake independent ontology development work. These efforts are often carried out within European Union-funded projects, for example under programmes such as Horizon 2020, as well as through institute-based research funding.

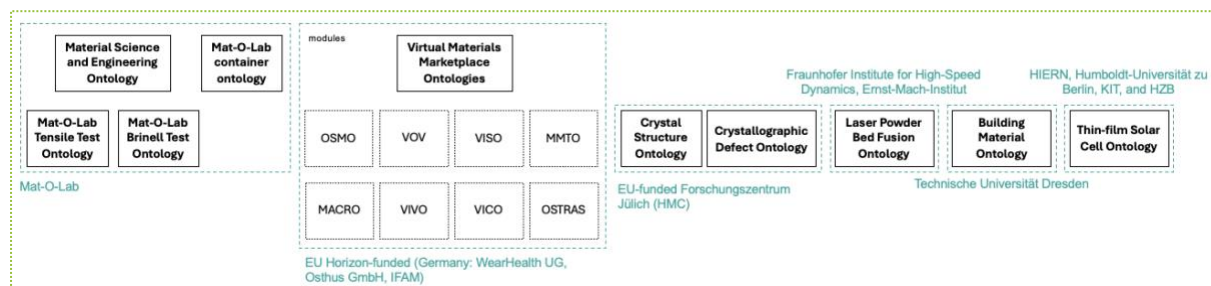


Figure 11: An overview of independent ontology initiatives

### Architecture and development process

The German approach to ontology architecture and development is characterised by a layered, standards-based ecosystem designed for long-term interoperability and sustainability:

- Basic Formal Ontology (BFO) is consistently adopted across major initiatives, providing architectural stability and enabling logical integration between independently developed domain ontologies.
- Dedicated mid-level backbone ontologies serve as shared semantic frameworks that accelerate cross-domain integration. These frameworks reduce duplication and ensure specialised ontologies remain interoperable through universally implemented modular architecture.

<sup>48</sup> Plattform MaterialDigital (PMD), *MaterialDigital* [online]. Available at: <https://www.materialdigital.de/>

- Application-level extensions provide sustainable growth pathways and enable domain specialisation without modifying or complicating foundational ontologies.

Professional engineering practices are systematically applied across the ontology ecosystem. Competency questions are commonly used to define the scope of ontologies, while the Ontology Development Kit (ODK) supports release management and version-controlled workflows across major initiatives. Automated validation routines further ensure logical consistency and maintainability. Explicit reuse of established ontologies is also a deliberate strategy, with widely adopted resources including PROV-O (Provenance Ontology), IAO (Information Artifact Ontology), OBI (Ontology for Biomedical Investigations), QUDT (Quantities, Units, Dimensions and Data Types Ontology), and EMMO (European Materials Modelling Ontology).

Open science governance is consistently practised across the ecosystem. Most ontologies are maintained in public GitHub repositories, and projects typically adopt open licences, such as Creative Commons Attribution 4.0 (CC BY 4.0) and the MIT License. Contribution mechanisms are usually documented, with some initiatives allowing open participation in development meetings and others relying on public pull-request review processes. This transparency helps build trust and encourages broader community adoption.

Ontology development is also frequently embedded within broader research infrastructure projects, integrating semantic modelling with repository architecture and workflow design. This ensures that ontologies remain closely connected to the tools that generate and consume research data rather than existing as abstract modelling exercises. At the same time, ontologies are subject to continuous curation and evolution. For example, the Basic Workflow for Materials Data (BWMD) ontology was modularised after its initial development, demonstrating that ontologies can be refactored and improved over time as requirements evolve.

### *Material types, industrial context and value chain coverage*

The resulting ecosystem spans multiple scales, material types, industry contexts, and value chain stages. It ranges from atomic-level ontologies for crystallographic defects, through process-level ontologies for steel and copper, to component-level ontologies for tensile testing, thereby enabling data continuity from fundamental science to engineering application.

Most ontologies developed in Germany that were identified in this report are material agnostic, while the second largest group focuses on crystalline materials.

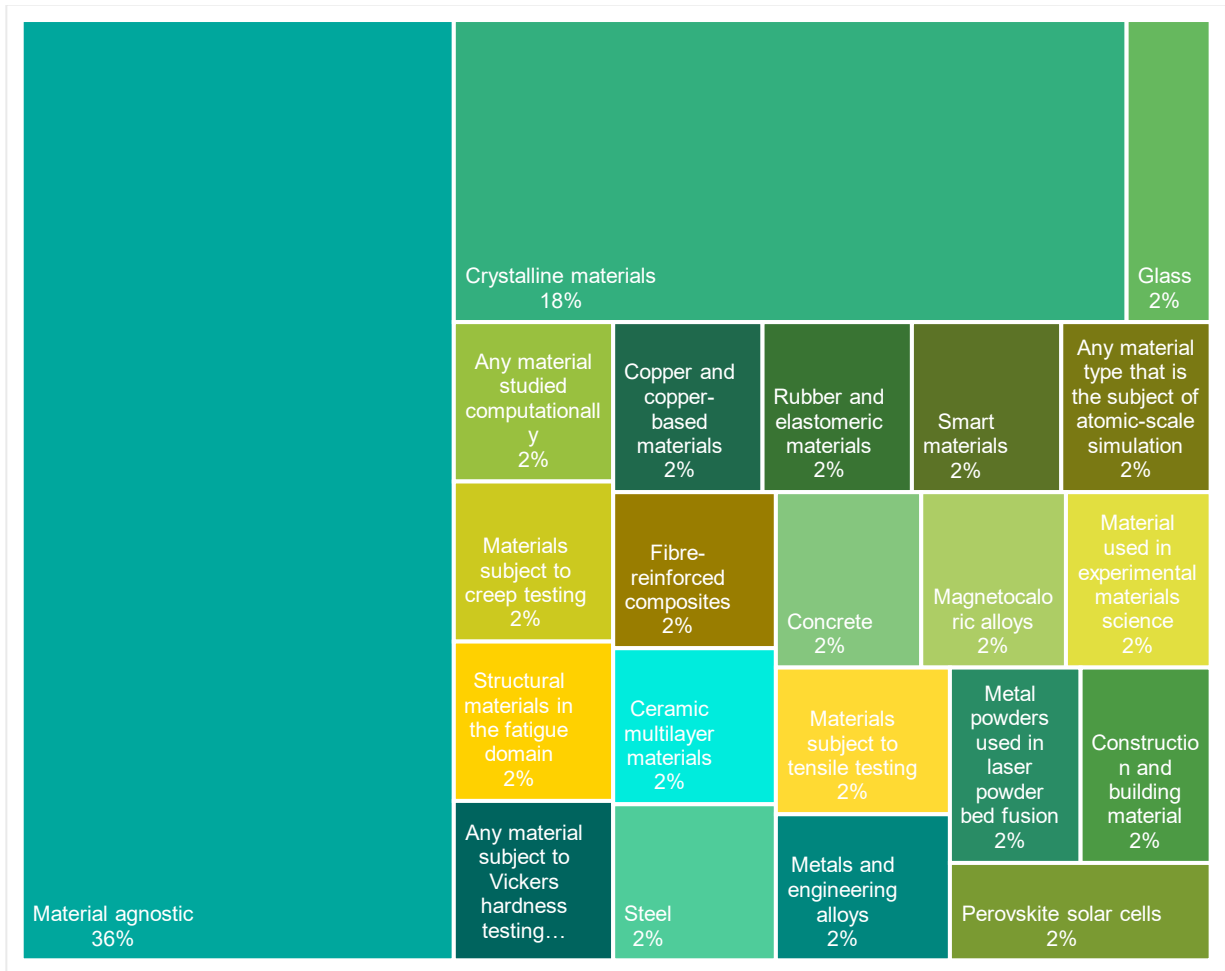


Figure 12: Ontologies developed in Germany (identified in this study) showed by material type focus.

Many ontologies cover more than one element of the materials value chain, with over 80% covering “Material and process discovery and design” and 75% “Synthesis, characterisation and metrology”.

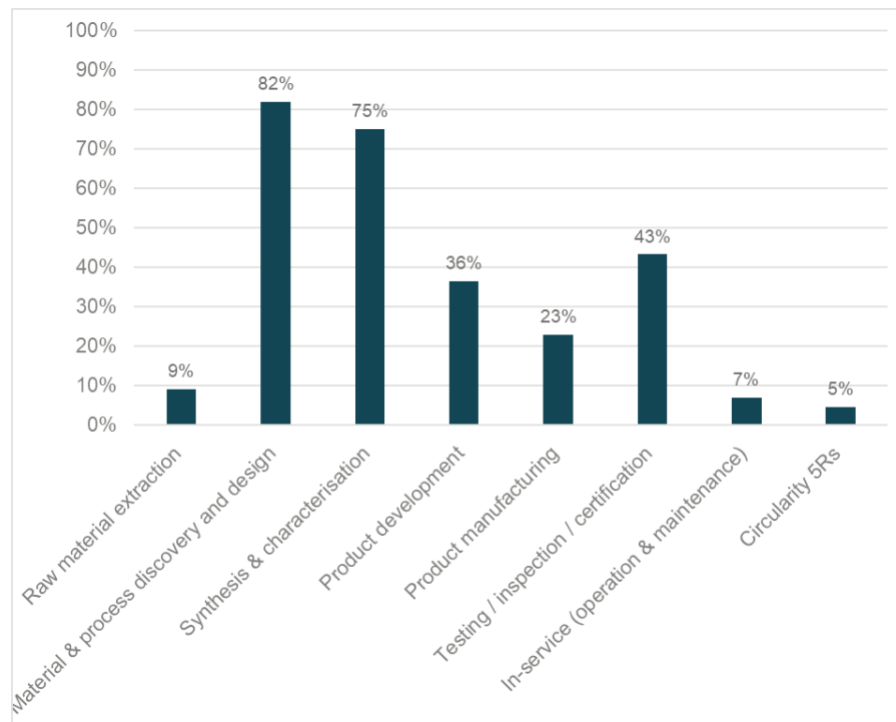


Figure 13: Ontologies developed in Germany, ordered by coverage across the materials value chain from upstream to downstream

### Key characteristics of the German approach

The review of over 40 ontology development initiatives highlights the following key characteristics of the German model:

1. **Coordinated funding that supports both disciplinary depth and cross-cutting interoperability.** Germany's combination of the National Research Data Infrastructure (NFDI), Platform MaterialDigital, and European Union funding enables deep domain expertise to develop alongside the frameworks needed to connect it.
2. **Funding of application ontologies alongside core infrastructure to create immediate value.** Platform MaterialDigital's support for copper, steel, and rubber ontologies demonstrates that practical use cases populate the ecosystem with operational data and encourage industry participation.
3. **Ontology development is embedded within infrastructure projects** to ensure ontologies address real requirements and evolve with the tools that consume data.
4. **Presence of common top-level framework**, e.g. Basic Formal Ontology (BFO), across the ecosystem. The consistent adoption of BFO across many German ontologies provides architectural stability and enables logical integration between independently developed ontologies.
5. **Investment in mid-level backbone ontologies** that domain projects can extend. In Germany case, National Research Data Infrastructure Core Ontology (NFDIcore) and the Platform MaterialDigital Core Ontology (PMDco) reduce duplication and ensure consistency by providing shared concepts that multiple domain projects can build upon rather than recreating from scratch.
6. **Application-level extensions enable active curation and further domain specification beyond initial development.** The modularisation of the Basic Workflow for Materials Data (BWMD) ontology, together with the Reference Datasets Ontology for Creep (RDOC) as an extension of the Reference Dataset Ontology (RDO), demonstrates that ontologies require planned pathways for growth beyond their original development stage.
7. **Designing for modularity** from the outset to enable independent development, selective reuse, and easier maintenance.
8. **Implementation of professional engineering practices**, including version control, competency questions, and automated validation. These methods help ensure that ontologies remain maintainable, auditable, and reproducible over time.
9. **Prioritisation of reuse of established ontologies** over developing concepts from scratch to minimises semantic divergence and ensures ecosystem integration.
10. **Open governance and clear contribution mechanisms.** Public GitHub repositories, open licenses, and documented contribution processes build trust and enable community participation across the ecosystem.

## Appendix 2: The value of Materials 4.0 in detail

**Limited evidence exists regarding the specific commercial and/or economic benefits that investment in Materials 4.0 delivers to the UK. This framework is accompanied by an evidence base of this potential opportunity.**

To begin building that evidence base, a series of in-depth interviews with strategically significant UK businesses involved in Materials 4.0 activity was conducted. The interviewees were senior representatives in businesses spanning metals, composites, polymers, battery materials, biocompatible materials and recycled materials. The sub-sections below provide a summary of key findings from the interviews, including that:

- Strategically significant UK businesses attach significant value, and are prepared to make major investments, into the capture and use of materials data.
- UK businesses quantify the value of materials data in varied and diverse ways, including everything from new revenue generation from materials data itself, through accelerated product development and product improvement, to avoiding the cost of product recalls and increased insurance premiums, and revenue creation from recycling.
- Materials data generates tangible commercial benefits across the entire materials value chain, including via raw material provenance, supply chain transparency and accountability, shorter material development and product development lead times, improved material and / or product performance, reduced expenditure on materials testing and verification, and higher-value options at end of life.
- Despite the significant value attached to materials data, the connection between investment in materials data and commercial returns is, understandably, often less well established given the complexity of the connection.
- There is unanimous agreement that a National Framework for Materials 4.0 would be utilised and could deliver further commercial opportunities, however, this was often contingent on acceptance of the data, models, simulations and results made available through the framework by end customers.
- Relatedly, many of the businesses interviewed recognised sensitivities associated with providing data inputs into a national framework. Most often these sensitivities were driven by non-disclosure agreements with end-customers, over and above any lack of willingness to input data into an appropriately governed national repository.

### Overview of commercial benefits

Every consultee confirmed that materials properties, performance, and data directly underpin their commercial operations – whether that is aeroengine performance cycles, catalytic activity for emissions control, biocompatibility of implantable electrodes, or the biodegradability timeline of packaging films.

Examples of the reported benefits of investment materials data are summarised in the table below and include: accelerated product development / improved time to market (most commonly cited); revenue generation and protection; safety, regulatory

compliance and risk reduction; cost reduction and process optimisation; sustainability and circularity; and supply chain resilience and market access.

Table 6: Summary of reported Materials 4.0 economic benefits across the full value chain.

Value chain element	Economic benefit types	Reported quantifiable benefits
<b>Raw material extraction</b>	Carbon reduction via recycled feedstock	6 - 16 vs 0.5 tonnes CO <sub>2</sub> /tonne for primary vs recycled aluminium
	Cheaper precursor selection through modelling	“Millions” saved on clean air products through data-driven precursor selection
<b>Material and process discovery and design</b>	Simulation replaces physical testing	“Hundreds of thousands of pounds” saved by modelling vs physical testing
	Research cycles cut by orders of magnitude	Product development accelerated by ~1 year through modelling
<b>Synthesis, characterisation and metrology</b>	Automated testing	Testing throughput increased from 10 to 50 tests/day (5x) through automation
	Safety data preventing costly plant upgrades	Over £5M saved by identifying alternative to volatile powder material before factory build
<b>Scale-up and material production</b>	Faster path to stable process design	18 months for supply chain NDA processes
	Data-driven grading of recycled feedstock at scale	10 - 20 £/tonne steel premium on millions of tonnes volume
<b>Product development</b>	Shared data compresses design cycles	Product development accelerated by ~1 year through modelling
<b>Product manufacturing</b>	Process monitoring prevents failure events	£10,000+ saved per commercial forming test
<b>Testing, inspection and certification</b>	Fraud detection via data	£1,000/kg vs £20/kg (PEEK fraud differential -- 50x)
	Regulatory data locks enables novel material use	~15% price uptick for biodegradable master batch at converter level

<b>In service (operations and maintenance)</b>	Digital passport enables traceability	>£100,000 loss every 2 days from resin failure
	Real-time performance tracking	material £30,000+ tank cleaning per incident
<b>Circularity 5Rs</b>	Materials enables recovery	passporting higher-value 8 - 9M tonnes steel scrap exported annually from UK as missed material value

The most common Materials 4.0 activities cited by interviewees included computational modelling and simulation, data platforms and data management, high-throughput experimentation, internet of things (IoT) monitoring and digital twins, and digital product passports. The focus of materials 4.0 activity was split between data attributes, digital infrastructure and materials data / AI models.

### Investment in Materials 4.0 activity

It was clear from the interviews that investment in Materials 4.0 activity is substantial, but that it is also difficult to quantify.

Interviewees consistently described their investment in materials data as significant but struggled to provide exact figures. Generally, the businesses interviewed invested in people, research and development activity and software licensing to enable their Materials 4.0 activity. For example, one interviewee indicated that the business spends “tens of millions of pounds on analytical equipment” for characterisation, and that their entire R&D function has data on its radar, including a big push currently on FAIR data principles.

A major UK recycling business reported a “huge amount of data and modelling work and digital twinning”, much of which was self-funded, and supplemented by Innovate UK grants and partner co-funding. The same business is currently building a major facility for bulk scrap measurement.

A composite materials developer runs its own testing labs as part of its service offering precisely because almost every new project requires bespoke materials testing from scratch.

All interviewees indicated growing investment in Materials 4.0, including investment in further integrating materials data into wider business processes, development of molecular-to-processing models, investment in in-process measurement and better understanding the value of existing materials data, and investment in shifting from iterative experimentation to data-driven approaches.

Public funding was seen as playing an important role in encouraging further Materials 4.0 activity. Strategically significant UK businesses have offered various letters of support for public investment in Centres for Doctoral Training (CDTs) to support Materials 4.0 related skills development, while several other interviewees referenced the role that Innovate UK funding played in supporting e.g., digital product passport feasibility studies, and co-funded materials 4.0 related research and innovation projects.

## Commercial motivations for Materials 4.0 investment

According to interviewees, the primary commercial drivers for investing in materials data span six interconnected themes:

- 1) Accelerated product development
- 2) Revenue generation and protection
- 3) Safety, regulatory compliance and risk reduction
- 4) Cost reduction and process optimisation
- 5) Sustainability and the circular economy
- 6) Supply chain resilience and market access

### **1) Accelerated product development and reduced time to market:**

- A specialty chemicals company reported that modelling has sped up product development by around a year in some cases, with potential savings of hundreds of thousands of pounds in development costs through reduced testing, and for larger products, savings running to millions by identifying cheaper precursors.
- A high-performance polymer company noted that generating validated material data cards through simulation rather than physical testing avoids spending tens of thousands of pounds on testing, particularly in the event that a customer decides not to proceed. Simulated testing reportedly takes hours, compared to months of physical testing.
- A composite materials developer indicated that design phases for aerospace applications can take over twelve months, while for automotive the full cycle from initial discussion to part production is three to four years in Europe. It was suggested that having a trusted data resource could save six months of groundwork, with the design phase estimated at ten to twenty per cent of total project cost. A second composite materials developer described materials data as an enabler without which they would not be able to sell parts or generate revenue, suggesting their technology could be a hundred times more effective with better access to materials data.
- A battery materials developer proposed that some battery companies failed partly because their R&D cycles were too long, and they could not reach a stable cell design quickly enough. AI was said to reduce these research cycle timelines by orders of magnitude, using relatively little data.
- A sustainable packaging producer noted that with fifteen degrees of freedom in their experiments, studying everything would require a billion experiments, and that data science approaches such as Bayesian optimisation allow targeted experimentation and faster product development.

### **Case study: QuesTek Innovations**

QuesTek Innovations is a commercial leader in Integrated Computational Materials Engineering (ICME).

Their Ferrium M54 steel – designed computationally using extensive materials databases – provides one of the most well-documented case studies of accelerated materials development. Ferrium M54 progressed from clean-sheet design to commercial production in approximately 4 years, with flight qualification within a further 3 years

(approximately 7 years total). This compares to a typical 15 – 20-year cycle for flight-critical alloy development and deployment.

The U.S. Navy estimated savings of ~\$3 million by implementing M54 steel in T-45 trainer aircraft hook shanks, which achieved more than 2x the service life of the incumbent alloy. Ferrium C64 gear steel for Army helicopters exceeded the 30-minute oil-out survivability requirement, lasting 85 minutes without failure. This directly reduces maintenance costs and prevents platform losses (a T-45 aircraft costs \$17.2M). The Ferrium M54 case was selected by NIST as a Quantitative Benchmark for Time to Market Framework case study, validating the Materials Genome Initiative (MGI) goal of new materials innovation in less than 10 years.

Source: [nist.gov](https://www.nist.gov)

## 2) Revenue generation and protection

- The materials informatics market is projected to grow from \$170m in 2025 to almost \$0.5bn by 2030 – a compound annual growth rate of over 19%. This growth is expected to be driven by increasing adoption of artificial intelligence and machine learning within materials science, continued acceleration of the materials research and development cycle, and growing demand for advanced materials across industries including but not limited to electronics, aerospace, automotive and healthcare<sup>49</sup>.
- A major aerospace business explained that aeroengine performance cycles – covering take-off, cruise and landing – are the metrics sold to airframers meaning materials data directly underpins this revenue stream. Thermal barrier coatings were offered as an illustration of this point – enabling combustion temperatures above the melting point of the underlying alloy, driving efficiency gains that determine competitive positioning in the market.
- A major UK recycling business noted that sophisticated recycled aluminium grades command a premium of two to three hundred pounds per tonne, while recycled steel carries a smaller premium of ten to twenty pounds per tonne but applies across millions of tonnes, meaning the aggregate value is substantial. Achieving these premiums depends on being able to characterise and verify the composition of recycled material, making materials data essential to unlocking higher-value recovery from end-of-life assets.
- An early-stage biomedical business noted that novel materials such as graphene-based electrodes represent a lucrative competitive position, but gaining regulatory approval requires substantial investment in materials data packages to demonstrate safety. Companies willing to make that investment could potentially secure significant first-mover advantage. The role that materials data plays in generating these sorts of competitive advantages was reiterated by other interviewees who also noted the importance of getting to market before competitors and that materials characterisation enables intellectual property protection and freedom to operate.

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<sup>49</sup> <https://www.marketsandmarkets.com/PressReleases/material-informatics.asp>

### 3) Safety, regulatory compliance, and risk reduction:

- A nuclear steels business noted that within the nuclear industry materials data is used to substantiate safety claims over very long service lives. Materials test results, certification records and inspection histories are used together to prove product longevity. Automation of data collection and transfer was seen as valuable because in the event of human error e.g., incorrectly noting the wrong tensile strength from a test certificate – in a nuclear context could have severe consequences. Hence, the accuracy and integrity of materials data within this, and other highly regulated industries is not just a quality issue but is also of paramount importance to safety.
- A specialty chemicals company reported that safety data on powder flammability, which showed a proposed new material to be unsafe, allowed for an alternative to be recommended and prevented a factory from needing a costly ATEX rating upgrade, potentially saving several million pounds.
- A materials and IoT data business highlighted how materials data enables algorithmic fraud detection and prevention. The interviewee cited documented cases of counterfeit bearings in aerospace, fake PEEK priced at fractions of the genuine cost, and the presence of mercury-based catalysts in resins, as examples of where absence of verified materials data has caused significant supply chain risk, potential safety failures and reputational exposure for the businesses involved.
- A biomedical technology business observed that regulatory data packages for novel implantable materials require enormous effort, money, and time, causing companies to default to already-approved materials and therefore effectively siffling the market for novel materials.
- A sustainable packaging business identified material failure in the supply chain (on the shelf) before the product's intended service life as the industry's key commercial risk, noting that as a perishable material, data on transient behaviour across different humidities, temperatures, and timelines is essential.

### 4) Cost reduction and process optimisation:

- An aerospace manufacturer explained that understanding material performance enables improvements to component quality, process optimisation, and cost reduction, with concessions data helping to improve supplier manufacturing processes.
- The materials data and IoT business reported that premature resin self-catalysis costs one customer six figures every two days, with single resin failure events costing well over a hundred thousand pounds and tank cleaning alone costing upwards of thirty thousand pounds.
- The major UK recycling business noted that primary aluminium produces six to sixteen tonnes of carbon dioxide per tonne compared with half a tonne for recycled aluminium, representing up to a thirty-two-fold reduction, while reuse steel achieves a thirty-eight-fold carbon dioxide reduction.
- The sustainable packaging business described how automating test analysis increased throughput from ten to fifty tests per day, a fivefold improvement.

### *Case study: Citrine Informatics*

Citrine Informatics, a leading materials informatics platform provider, reports that its AI-driven sequential learning approach can reduce the number of experiments needed for product development by 50–80%.

Documented applications include:

**Aerospace alloy development:** In collaboration with HRL Laboratories, Citrine’s platform searched through 11.5 million combinations of powders and nanoparticles to identify 100 optimised candidates, resulting in AL 7A77, the first high-strength aluminium alloy powder feedstock for off-the-shelf additive manufacturing machines. The first commercial customer was NASA Marshall Space Flight Centre.

**Autonomous nanoparticle synthesis:** In collaboration with SLAC National Accelerator Laboratory, Citrine built a closed-loop autonomous system that reached multiple design objectives in just 12 hours, starting with no historical data.

**Custom composite materials:** Working with Siemens Digital Industries Software, Citrine’s platform enabled rapid identification of custom polymer blends meeting customer-specific performance targets with far fewer experiments than traditional approaches.

Source: [citrine.io](https://citrine.io)

### *5) Sustainability and the circular economy:*

- The major UK recycling business suggested that the carbon and resource security arguments for recycled materials are compelling, noting that the UK exports roughly eight to nine million of approximately ten million tonnes of steel scrap annually for low-grade use, while at the same time importing primary steel, and that nearly all freely available aluminium leaves the country.
- The materials data and IoT business highlighted that recyclers cannot determine correct pathways without knowing what materials are in products, citing the example of wind turbine blades having thirteen components (compared to the four declared), and noting that greenwashing legislation is expected to have real enforcement power.
- The battery materials research interviewee highlighted that battery passports providing traceability, carbon footprint data, and recycling instructions via QR codes are very important to the wider battery space commercially.
- The biomedical technology company suggested that better materials data could lead to devices with less environmental impact that do not need to be replaced as often.

### *Case study: Rolls-Royce*

Rolls-Royce has implemented the Ansys Granta materials information (MI) management system.

Rolls-Royce deployed Granta MI as a “gold source” of verified materials information, accessible to over 2,000 engineers globally across its civil, defence, and nuclear businesses. Certified savings of several million dollars per annum were reported, in time saved, process optimisation and reduced waste. Key drivers of these savings included: reduced duplication of mechanical testing; improved traceability and compliance in a

highly regulated environment; and better-informed materials decisions feeding into design and simulation.

Source: [ansys.com](https://www.ansys.com)

#### **6) *Supply chain resilience and market access:***

- The materials and IoT business reported that tier one manufacturers are starting to demand manufacturing data from suppliers, driven by legislation, and that insurance disputes are arising where companies cannot prove material provenance.
- A composites developer noted that customers in Europe are very sensitive about what information they share, and that a majority of testing data is locked under non-disclosure agreements, fragmenting the industry knowledge base.
- The UK recycling business observed that knowing what materials are in buildings, wind turbines, and other assets before end of life enables pre-marketing and higher-value recovery.

## Appendix 3: Stakeholder engagement details

### Survey questions

For each of the seven challenges – presented with the same descriptions as on page 45 – respondents were asked:

1. Where does this challenge present a barrier? (Please select all that apply.)  
Descriptions of these value chain elements can be found in the interim report: [https://www.royce.ac.uk/wp-content/uploads/2025/12/Henry\\_Royce\\_Institute\\_Materials\\_4\\_0\\_Framework\\_InterimReportWebsite.pdf](https://www.royce.ac.uk/wp-content/uploads/2025/12/Henry_Royce_Institute_Materials_4_0_Framework_InterimReportWebsite.pdf)
  - a. Raw material extraction
  - b. Material and process discovery and design
  - c. Synthesis, characterisation and metrology
  - d. Scale-up and material production
  - e. Product development
  - f. Product manufacturing
  - g. Testing, inspection and certification
  - h. In service (operations and maintenance)
  - i. Circularity (5Rs)
2. What short-term (2026 – 2027) actions do you perceive are required to address this challenge?
3. What medium-term (2028 – 2030) actions do you perceive are required to address this challenge?
4. What long-term (2030 onwards) actions do you perceive are required to address this challenge?
5. What enablers are needed for these actions? I.e., specific funding, skills, resources, partnerships, or capabilities.
6. Do you know any examples from other industries where this challenge has been overcome?

In a closing section, respondents were asked:

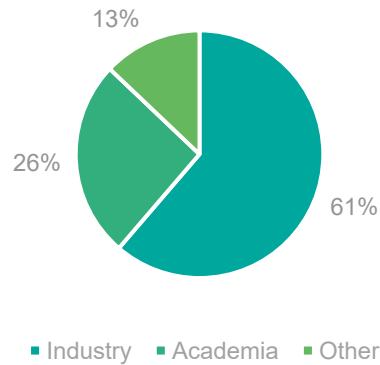
1. Based on your experience, please rank the challenges from 1 (highest priority) to 7 (lowest priority).
2. Do you have any further comments on the challenges and potential actions to accelerate Materials 4.0 adoption in the UK?

### Survey respondents

The survey gathered 31 responses between 12<sup>th</sup> and 26<sup>th</sup> February 2026, from stakeholders across academia, industry and government. The survey questions and full responses are in Appendix 2.

The survey was a crucial opportunity to reflect the views of the materials community on actions to facilitate and promote Materials 4.0 adoption. It was successful in capturing input from a range of industry, academia and others.

### Respondents' Background



### Workshop agenda

- Intro and into break outs 5 mins
- First challenge:
- Review and discuss the survey responses 10 mins
  - Vote for high-priority actions 2 mins
- Draft challenge-based roadmaps together 20 mins
- Second challenge:
- Review and discuss the survey responses 10 mins
  - Vote for high-priority actions 2 mins
- Draft challenge-based roadmaps together 20 mins
- Present back to the wider group 20 mins

### Survey and workshop results

*Challenge 1: Interoperability and shared semantics (ontologies, schemas, and identifiers)*

Actions (clustered)

Actions suggested	per timescale
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Cluster	Definition	Short-term (2026 - 2027)	Medium-term (2028 - 2030)	Long-term (2030 onwards)
Stakeholder Convening, Governance & Working Groups	Creation of expert groups, governance bodies, and coordinated national/international stakeholder forums to steer semantic alignment.	7	6	2
Semantic Assets: Dictionaries, Controlled Vocabularies & Ontologies	Development, synchronization, and governance of materials dictionaries, vocabularies, and ontologies.	6	4	4
Reporting Standards & Minimum Information Schemas	Defining and standardizing materials property reporting formats, codes, and minimum metadata requirements.	3	3	2
Landscape Mapping, Terminology Audits & Harmonisation	Auditing current terminology, mapping datasets, identifying inconsistencies, and harmonising definitions.	4	1	1
Training, Education & Change Management	Training users on standards, structuring data, and long-term change management for adoption.	3	2	2
Pilots, Demonstrators & Adoption Pathways	Running pilots and demonstrators to validate data standards and interoperability in real industrial chains.	1	1	1
Infrastructure: Digital Pipelines, Databases & Interoperable Platforms	Developing shared databases, APIs, digital twins, national data backbones, and interoperable platforms.	0	5	2
Vendor & Equipment Manufacturer Integration	Ensuring vendors and equipment support standardised outputs and automated data capture.	1	2	2

Legislation, Accreditation & Policy Levers	Mandates, accreditation systems, ISO standards and regulatory levers to institutionalise semantic interoperability.	0	1	3
AI-enabled Semantic Quality Assurance & Automation	Use of AI and automation to validate standards, generate structured data, and automate workflows.	0	3	2
Long-term Maintenance of Semantic Assets	Sustained governance and maintenance of ontologies and dictionaries via formal approval bodies.	1	1	2

#### Enablers (clustered)

Cluster	Definition	Quantity of suggestions
Funding & Financial Support	Sustained funding for standards development, infrastructure, open-source tools, skills programmes, and cross-sector collaborations.	13
International Alignment & Standards Harmonisation	Coordination of global materials suppliers, participation in international standards bodies, harmonisation across regions to avoid local silos.	6
Cross-sector Partnerships & Collaboration	Partnerships across industry, academia, government, SMEs, and international agencies to co-develop standards and shared data languages.	7
Skills, Training & Community Building	Building skills in data engineering, ontology development, materials semantics, coding, and providing user training and community development.	6
Leadership, Governance & National Coordination	Strong national leadership, governance structures, and mandated coordination to align semantic efforts across sectors and ensure stewardship.	5
Tooling, Infrastructure & User Interfaces	Investment in databases, digital infrastructure, user interfaces, and tools that simplify data entry, validation, and semantic compliance.	4

## Workshop voting outcome

Votes	Action Cluster
4	Long-term Maintenance of Semantic Assets
3	Different requirements of interoperability between different organisations, especially small companies
3	Semantic Assets: Dictionaries, Controlled Vocabularies & Ontologies
3	Infrastructure: Digital Pipelines, Databases & Interoperable Platforms
2	Training, Education & Change Management
2	AI-enabled Semantic Quality Assurance & Automation
1	Awareness of existing standards, especially open source and semantics that can be used for Materials 4.0
1	Landscape Mapping, Terminology Audits & Harmonisation
1	Reporting Standards & Minimum Information Schemas
1	Stakeholder Convening, Governance & Working Groups
0	Pilots, Demonstrators & Adoption Pathways
0	Legislation, Accreditation & Policy Levers
0	Vendor & Equipment Manufacturer Integration

## Challenge 2: Data availability, quality, and “FAIR-ness”

Actions (clustered)

Cluster	Definition	Actions suggested per timescale		
		Short-term (2026 - 2027)	Medium-term (2028 - 2030)	Long-term (2030 onwards)
FAIR Training, Culture & Behaviour Change	Training, education, and cultural change to promote FAIR data practices, metadata use, sharing of negative data, and improved data hygiene.	7	6	4
Metadata Standards, Quality Criteria & Reporting Rules	Creation and adoption of minimum metadata requirements, data quality standards, reporting rules, and lifecycle information standards.	5	8	5

Data Discovery, Dark Data Recovery & Auditing	Identification, auditing, and recovery of dark data, assessment of legacy datasets, and decisions on cleaning versus new data generation.	4	1	1
FAIR Infrastructure, Repositories & Interoperable Systems	Creation and scaling of shared repositories, databases, FAIR-by-design pipelines, ELNs, digital twins, and long-term national/international data infrastructure.	1	5	5
Partnerships, Consortia & Cross-sector Collaboration	Consortia, cross-sector partnerships, collaboration between data holders, journals, funders, and regulatory bodies to support FAIR implementation.	3	5	4
Governance, Regulation & Incentives	Mandates, regulatory frameworks, incentives, and governance mechanisms to enforce FAIR adoption and long-term stewardship.	3	4	5
New Data Generation & Prioritisation	Guidance on when to regenerate datasets, selection workflows, prioritisation, and establishing high-quality new datasets.	2	1	2

#### Enablers (clustered)

Cluster	Definition	Quantity of suggestions
Funding & Sustained Investment	Long-term funding for FAIR infrastructure, data stewards, ELNs, curation, software, skills programmes, SME participation, and cross-industry initiatives.	14
Skills, Training & Workforce Development	Skills development in data management, FAIR principles, ELNs, metadata standards, STEPs standards, ontology use, and cultural change towards sharing.	10
Governance, Regulatory & Standards Bodies	Regulators, international standards organisations, certification mechanisms, and governance for data access, metadata requirements, and trusted frameworks.	8

Partnerships, Consortia & Cross-sector Collaboration	Collaboration between academia, industry, government, journals, circularity experts, regulatory bodies, SMEs, repositories and infrastructure operators.	12
Infrastructure, Tools & Technology (ELNs, STEP, Cloud, Metadata Systems)	Technical infrastructure such as ELNs, cloud systems, STEP-based tools, metadata schemas, data pipelines, curation tools, scraping certifications, and repository restoration.	8

### Workshop voting outcomes

Votes	Action Cluster
5	Metadata Standards, Quality Criteria & Reporting Rules
4	FAIR Infrastructure, Repositories & Interoperable Systems
3	Data Discovery, Dark Data Recovery & Auditing
2	Governance, Regulation & Incentives
1	New Data Generation & Prioritisation
0	Partnerships, Consortia & Cross-sector Collaboration
0	FAIR Training, Culture & Behaviour Change

### Challenge 3: IP, cybersecurity, and governance across multi-stakeholder ecosystems

#### Actions (clustered)

Cluster	Definition	Actions suggested per timescale		
		Short-term (2026 - 2027)	Medium-term (2028 - 2030)	Long-term (2030 onwards)
IP Identification, Protection & Minimisation of Shared Information	Actions focused on defining protected IP, limiting information shared, enforcing ownership clarity, and understanding disclosure risks.	6	4	3
Governance Frameworks,	Rules, standards, governance models, auditability requirements, contractual	4	6	4

Regulations & Policy Harmonisation	structures, and global IP/data-sharing alignment.			
Secure Collaboration Environments	Trusted Research Environments (TREs), encrypted sharing channels, secure data rooms, federated platforms, and sandpit environments.	4	5	2
Access Control, Authentication & Tiered Permissions	Multi-factor authentication, granular permissions, metadata-only visibility, and role-based access systems.	4	3	3
Federated Learning & Privacy-Preserving Technologies	Using federated machine learning, secure computation, and technologies enabling insights without exposing sensitive data.	1	1	1
Training, Awareness & Culture Change	Training on IP management, data-sharing best practices, risk-awareness, and trust-building across supply chains.	4	1	0
Incentives, Investment & Motivation Structures	Incentives for sharing, funding requirements, speeding IP approval, and investment in enabling tools and platforms.	3	4	1
Challenges, Barriers & Scepticism About Feasibility	Expressions of difficulty, legal resistance, or unwillingness to share IP even with safeguards.	3	1	1

#### Enablers (clustered)

Cluster	Definition	Quantity of suggestions
Funding, Resources & Investment	Need for financial support, dedicated resources, neutral environments, insurance mechanisms, and investment in secure digital infrastructure.	6
Training, Skills & Awareness	Developing skills in IP, trade secrets, cybersecurity, digital trust, and data governance across academia, industry, and supply chains.	5
Standards, Frameworks & Legal Structures	Development of national IP guidance, legal frameworks, standards, standardised methodologies, and	3

	contracts enabling data sharing and co-development.	
Expertise & Specialist Support	Requirement for IT, cybersecurity, regulatory and data experts, as well as partnerships with organisations demonstrating best practice.	3
Trust, Collaboration & Cultural Change	Building understanding of the value of data sharing, creating trusted brokers, enabling collaborations, and assessing risk-benefit trade-offs.	4

### Workshop voting outcomes

Note that there were two rounds of voting in this challenge, as the first resulted in a tie.

Votes	Action Cluster
3 (+4)	Secure Collaboration Environments
3 (+2)	IP Identification Protection & Minimisation of Shared Information
3 (+2)	Challenges, Barriers & Scepticism about Feasibility
3	Governance Frameworks, Regulations & Policy Harmonisation
3	Training, Awareness & Culture Change
2	Access Control, Authentication & Tiered Permissions
2	Federated Learning & Privacy-Preserving Technologies
1	Incentives, Investment & Motivation Structures
1	Who has the authority to make decisions?

### Challenge 4: Model credibility: uncertainty quantification, validation, and “physics vs. black box”

Actions (clustered)

Cluster	Definition	Actions suggested per timescale		
		Short-term (2026 - 2027)	Medium-term (2028 - 2030)	Long-term (2030 onwards)

Model Validation, Credibility & Uncertainty Quantification	Activities focused on validating models against physical data, defining credibility requirements, establishing benchmark datasets, and improving traceability and uncertainty quantification.	3	4	3
Digital Twins, Physical–Virtual Integration & Sensor Connectivity	Improving integration between physical processes and digital twins, identifying where digital twins are needed, enhancing data flows, and developing hybrid models.	3	2	2
TRL Advancement, Industry–Academia Collaboration & Embedding	Bridging the TRL valley of death, embedding researchers across sectors, building joint projects, and developing industrially relevant demonstrators.	3	4	3
Sector-Specific Modelling Needs (Nuclear, Composites, High-Value Materials)	Actions tied to nuclear materials modelling, composites shape–structure relationships, and specialised modelling requirements for safety-critical sectors.	3	2	2
Infrastructure, Data Trust & Shared Environments	Building data environments, secure shared platforms, and establishing trust needed for cross-organisation model usage.	3	1	0
Model Deployment, Scaling & Operational Integration	Ensuring models can scale, be deployed in production settings, integrating VV/UQ tools, and ensuring long-term workflows.	2	1	2

#### Enablers (clustered)

Cluster	Definition	Quantity of suggestions
Funding, Resources & Investment	Funding streams, focused investment across TRLs, headcount, and support for innovation centres.	4
Expertise, Skills & Competence Development	Skills in modelling, validation, metrology-aware data engineering, applied ML, and sector-specific modelling expertise.	4
Standards, Benchmarking &	Benchmark datasets, shared test structures, standardised validation and	1

Validation Frameworks	uncertainty quantification protocols, metadata standards.	
Collaboration, Communication & Sector Alignment	Improved academia–industry communication, cross-sector champions, secondments, and shared understanding of industrial context.	3
Use Cases, Applicability & Knowledge Transfer	Creation and dissemination of use cases, applicable R&D, and demonstration of industrial relevance.	2
Model Scalability & Design for Industrial Use	Ensuring models are designed for scalability, operational fit, and transition from research to industrial environments.	1

### Challenge 5: Reliable automated labs and computing power requirements

Actions (clustered)

Cluster	Definition	Actions suggested per timescale		
		Short-term (2026 - 2027)	Medium-term (2028 - 2030)	Long-term (2030 onwards)
Funding, Infrastructure & Investment	Funding for scaling, demonstrators, automation equipment, and long-term investment in engineering capability and high-throughput experimentation infrastructure.	6	3	1
Collaboration, Communication & TRL Bridging	Cross-sector collaboration, engagement between engineers and microscale specialists, academia-industry communication, and bridging the TRL gap for scale-up.	4	4	2
Standards, Protocols &	Development of standards, process verification frameworks, uncertainty protocols, auditability, reliability	2	2	2

Verification Frameworks	requirements, and long-term automation certification.			
Modular Automation, Interoperability & Workflow Integration	Modular equipment design, interoperable systems, transferable workflows, API standards, metadata structure, and automation frameworks.	3	3	2
Data Integration, Feedback Loops & Digital Twins	Reliable data feedback from applications, integration of sensor and process data, higher-variation modelling, and development of realistic digital twins.	2	1	2
Understanding Barriers, Prioritisation & Strategic Planning	Mapping gaps, identifying bottlenecks, prioritising value chains, developing action plans, and determining when automation is genuinely needed.	3	3	0

#### Enablers (clustered)

Cluster	Definition	Quantity of suggestions
Funding, Investment & Risk Mitigation	Substantial funding for retrofitting automation, mitigating TRL valley-of-death risks, business restructuring, and incentives for scalable automation.	5
Cross-Sector Collaboration, Forums & Knowledge Exchange	Cross-sector learning, sandpits or forums, collaboration between automation and characterisation specialists, and industry benchmarks.	4
Skills, Expertise & Workforce Capability	Skills to design scalable automated systems, regulatory and IT expertise, materials–metrology–software integration skills, and SMEs with scale-up expertise.	4
Standards, Interoperability & Automation Frameworks	Interoperable metadata standards, APIs, vendor cooperation, secure orchestration platforms, workflow QA, version control, and reliability engineering.	1

High-Quality Production Data & Benchmarking	Generation of high-quality annotated production data to understand differences between lab and production scale and support automation scaling.	1
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**Challenge 6: Qualification, standards, and regulatory acceptance (especially for safety-critical materials)**

Actions (clustered)

Cluster	Definition	Actions suggested per timescale		
		Short-term (2026 - 2027)	Medium-term (2028 - 2030)	Long-term (2030 onwards)
Mapping Standards, Frameworks & Regulatory Landscape	Identifying existing standards, mapping gaps, understanding regulatory regimes, and establishing harmonised rules and cross-sector alignment.	10	7	3
Qualification Pathways, Validation & Uncertainty Quantification	Developing qualification-aligned workflows, uncertainty quantification tools, test structures, pilot validation pathways, and parallel testing.	3	3	3
Dialogue, Engagement & Stakeholder Confidence	Dialogue with regulators, building stakeholder understanding, engagement with standards bodies, and clarifying regulatory processes.	4	2	2
Education, Skills & Capability Development	Skills development in regulatory processes, qualification, materials data standards, model acceptance, and integration of these topics into academic curricula.	2	3	2
Cross-Sector Use Cases, Reference Cases & Shared Infrastructure	Building shared datasets, cross-sector databases, round-robin studies, and using lower-regulation sectors as stepping stones for qualification.	1	2	1

Innovation Culture, Model Adoption & Digital Transformation	Adoption of explainable AI, physically informed models, fail-fast innovation culture, and shifting organisational practices to accept digital evidence.	2	3	2
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Enablers (clustered)

Cluster	Definition	Quantity of suggestions
Cross-Sector Collaboration & Regulatory Alignment	Collaboration across sectors and jurisdictions, joint action with regulators, harmonisation of requirements, and recognition of shared qualification needs.	3
Safety, Risk Management & Regulatory Integrity	Maintaining rigorous safety expectations, integrating risk-benefit analysis, ensuring ML/digital tools meet existing safety standards, and leveraging regulatory SMEs and lobbyists.	3
Standards Development, Auditability & Qualification Infrastructure	Standards bodies engagement, benchmark datasets, round-robin validation, digital auditability, model cards, traceability, and sustained investment in standards creation.	3
Expertise, Skills & Regulatory Science Capability	Development of skills in standards, regulatory science, auditing, safety-critical model use, agile/lean approaches, and interdisciplinary technical expertise.	3
Funding, Resources & Organisational Capacity	Funding for qualification pilots, standards activities, regulatory validation, restructuring, and long-term capability building in companies and research ecosystems.	4

## Challenge 7: Incentives (including economic), culture, skills, and organisational change

Actions (clustered)

Cluster	Definition	Actions suggested timescale		
		Short-term (2026 - 2027)	Medium-term (2028 - 2030)	Long-term (2030 onwards)
Skills Development, Training & Hybrid Competence	Development of interdisciplinary skills blending materials science, data science, automation, software, and statistics; creation of training programmes, academies, curriculum changes, and national skills frameworks.	9	7	3
Culture Change, Organisational Transformation & Incentive Structures	Shifting organisational culture to value data stewardship, software-like practices, and long-term digital transformation; creating incentives, business cases, leadership programmes, and organisational capacity for change.	6	5	4
Cross-Sector Collaboration, Best Practice Sharing & Communities of Practice	Mechanisms enabling shared learning, cross-industry collaboration, best practice exchange, and adoption of approaches from adjacent sectors (pharma, US initiatives, HE, etc.).	6	3	3
Infrastructure, Compute Access & Tools for Scalable Digital Working	Provision of accessible compute resources, easy-to-use data management tools, FAIR/semantic data systems, and software environments that reduce overhead and support digital working at scale.	3	2	1
Recruitment, Workforce Expansion & Professionalisation	Hiring specialists, protecting existing skilled staff, establishing professional roles such as Data Manager, and creating long-term workforce pipelines.	1	2	1

## Enablers (clustered)

Cluster	Definition	Quantity of suggestions
Funding, Investment & Organisational Capacity	Long-term funding, structural investment, company restructuring, and financial mechanisms that support sustained Materials 4.0 transformation.	6
Skills, Training & Workforce Development	Development of digital, automation, and hybrid materials–software skills through training programmes, curricula changes, and career pathways.	4
Digital Infrastructure, Platforms & Tools	Automation capabilities, no-code platforms, chemically aware tools, equipment, and FAIR-compliant digital environments enabling scalable Materials 4.0 adoption.	2
Standards, Regulation & Governance Support	Business experts, regulatory experts, and governance mechanisms supporting responsible adoption and qualification of digital materials workflows.	2
Cross-Sector Partnerships, Consortia & Community Building	Industry–academia partnerships, neutral convening organisations, consortia formation, and knowledge-sharing communities to accelerate adoption.	2

## Workshop voting outcomes

Votes	Action Cluster
5	Economic Incentives & Funding
4	Infrastructure, Compute Access & Tools for Scalable Digital Working
2	Skills Development, Training & Hybrid Competence
2	Cultural Change, Organisational Transformation & Incentive Structures
2	Cross-Sector Collaboration, Best Practice Sharing & Communities of Practice
0	Recruitment, Workforce Expansion & Professionalisation

## Implementation roadmaps

The top four cross-sector challenges were processed in a co-creation workshop. The four highest-priority challenges were selected for further analysis and specific actions were proposed to address each challenge. The participants prioritised the actions and selected the most important one to develop into an implementation roadmap – compiling suggested activities into snapshots for action. The four roadmaps derived are shown in the section below.

## Data availability, quality and “FAIR-ness”

### Metadata Standards, Quality Criteria & Reporting Rules

Creation and adoption of minimum metadata requirements, data standards, reporting rules and lifecycle information standards.

	WHEN?			VISION	
	Short-term (2026)	Medium-term (2027-2030)	Long-term (2030+)	What success looks like?	does look like?
WHY? Benefits and drivers Where in the value chain?	<ul style="list-style-type: none"> <li>Knowing whether the data exists is essential to knowing whether it's of value.</li> </ul>	<ul style="list-style-type: none"> <li>Harnessing/generating value from data.</li> <li>Infrastructure, Tools &amp; Technology (ELNs, STEP, Cloud, Metadata Systems)</li> </ul>		Structure of the metadata (alignment with ontology) that spans the whole life-cycle of the materials.	
WHAT? Key activities Key digital elements	<ul style="list-style-type: none"> <li>Develop gold standard for metadata generation and management.</li> <li>Exemplar/demonstrators</li> <li>Data fidelity – mandate via UCAS?</li> <li>Mandate to do so at higher level? Or an organisation taking the initiative to lead/be incentivised to lead.</li> </ul>	<ul style="list-style-type: none"> <li>Deep expertise requirements in data science.</li> <li>Deep expertise requirements in materials science.</li> </ul>		Flexibility to tackle different materials and combination of materials.	
WHO? Stakeholders across industry, academia and government	<ul style="list-style-type: none"> <li>Governance, Regulatory &amp; Standards Bodies</li> <li>Hartree, Diamond Light, Liverpool, Imperial (high throughput labs)</li> </ul>			Adaptability and evolution of the metadata based on technological advances.	
				Linked to	

	<ul style="list-style-type: none"> <li>National Center for Advanced Materials Performance (NCAMP) – platform of trusted data (<a href="#">link</a>)</li> </ul>			<p>manufacturing data practices/systems</p>
<p>HOW?</p> <p>Size of the funding required</p> <p>Skills, partnerships and structures</p>	<ul style="list-style-type: none"> <li>Funding &amp; Sustained Investment</li> <li>Skills, training &amp; Workforce Development</li> <li>Partnerships, Consortia &amp; Cross-sector Collaboration</li> <li>Governance, Regulatory &amp; Standards Bodies</li> </ul>			<p>Working towards integrated contexts.</p>

## Incentives (including economic), culture, skills, and organisational change

### Economic Incentives & Funding

Data, tools, methods and techniques could be valuable for different applications if it is well annotated. Materials data as a business model/revenue stream.

	WHEN?			VISION
	Short-term (2026)	Medium-term (2027-2030)	Long-term (2030+)	What does success look like?
<b>WHY?</b> Benefits and drivers Where in the value chain?	→ Increase data quality → Increase data sharing practices	→ Realise economic value from existing data	→ Develop other business models/revenue streams	Structural recognition of the value of data and models, incentivising stakeholders to engage more in data/model curation and sharing.  Data becomes increasingly better, leading to better value generation from the data shared.  Developing a UK economy segment to extract value of materials data/models (e.g., satellites for surveying/Earth observation).
<b>WHAT?</b> Key activities Key digital elements	→ Understanding the economic context of data → Diagnostic of the breakdown between sharing small vs large amounts of data (capitalisable) → Critical amount of data for unlocking value in large pool of data → Understanding the quality needs of data at specific levels	→ Voucher schemes to discover internal materials data, produce metadata		
<b>WHO?</b> Stakeholders across industry,	→ UKIPO as benchmark for insights → Data/model creators → Broader stakeholders from fields			

academia and government				QUBIS example (Queensland university datasets, in bio-molecule space), data was public/IP, gets capitalised on by companies Google/people's data (critical mass data levels)
HOW? Size of the funding required Skills, partnerships and structures	<ul style="list-style-type: none"> <li>→ Funding, Investment &amp; Organisational Capacity</li> <li>→ Skills, Training &amp; Workforce Development</li> <li>→ Digital Infrastructure, Platforms &amp; Tools</li> <li>→ Standards, Regulation &amp; Governance Support</li> <li>→ Cross-sector Partnerships, Consortia &amp; Community Building</li> </ul>			

## Interoperability and shared semantics

### Long-term Maintenance of Semantic Assets

Sustained governance and maintenance of ontologies and dictionaries via formal approval bodies.

	WHEN?			VISION
	Short-term (2026)	Medium-term (2027-2030)	Long-term (2030+)	What does success look like?
<b>WHY?</b> Benefits and drivers Where in the value chain?				Establishing ease of access, ease of use and preserving ontologies for the long term, through collaborative partnerships of different organisations.  Could be either a community of practice, industry body, government department or a single entity e.g. national or international standards body depending on the application.
<b>WHAT?</b> Key activities Key digital elements	<ul style="list-style-type: none"> <li>→ Identify some specific use cases (either from large user/industry or community-led) where the value can be demonstrated</li> <li>→ Educated different communities and demonstrate the value of shared ontologies</li> <li>→ Look at established current databases to establish relevant</li> </ul>	<ul style="list-style-type: none"> <li>→ Easy access to experts so SMEs can navigate and adopt a complex technical area (data) which might not be their level of expertise</li> <li>→ International alignment &amp; standards harmonisation - coordination of global materials suppliers, participation in international standards bodies,</li> </ul>	<ul style="list-style-type: none"> <li>→ Sustained governance and maintenance of ontologies and dictionaries via a community of practice, industry body, government department or a single entity, e.g. national or international standards body, depending on the application</li> </ul>	

	collaborations with industrial partners	harmonisation across regions to avoid local silos – perhaps AI can help harmonise data between different national standards		
WHO? Stakeholders across industry, academia and government				
HOW? Size of the funding required Skills, partnerships and structures	<ul style="list-style-type: none"> <li>→ Funding for supporting community-led use case development</li> <li>→ Cross-sector partnerships and collaboration</li> <li>→ Skills, training and community building – building skills in data engineering, ontology development, materials semantics, coding and providing user training and community development</li> </ul>	<ul style="list-style-type: none"> <li>→ It's more of change management and support to organisations rather than a technical challenge</li> </ul>		

*IP, cybersecurity, and governance across multi-stakeholder ecosystems*

**Shared Collaboration Environments**

**Secure environments for both data, infrastructure and hazardous materials**

	WHEN?			VISION
	Short-term (2026)	Medium-term (2027-2030)	Long-term (2030+)	What does success look like?
<p>WHY?</p> <p>Benefits and drivers</p> <p>Where in the value chain?</p>	<p>Potentially three streams:</p> <ol style="list-style-type: none"> <li>1. commercially sensitive / trade secrets</li> <li>2. customer/user data (GDPR)</li> <li>3. data products</li> </ol> <p>Perhaps the solution is to have metadata to describe the category 1 data</p>			<p>Trusted Research Environments (TREs), encrypted sharing channels, secure data rooms, federated platforms, and sandpit environments.</p> <p>Federated learning for AI models that have been developed.</p> <p>Note: Federated learning is transfer the learning from AI models and combine them with other AI models that had similar training.</p>
<p>WHAT?</p> <p>Key activities</p> <p>Key digital elements</p>	<ul style="list-style-type: none"> <li>→ Small pilot in a non-critical area that uses non-critical data to test and ensure that data is secure.</li> <li>→ Learning from other sectors e.g. fintech and pharma/biotech/defence/software industry/logistics that have successfully demonstrated secure data sharing</li> <li>→ National cyber-security lab providing advice to smaller companies</li> </ul>	<p>Knowledge transfer from experts to the M4.0 pilot(s)</p>		

	<ul style="list-style-type: none"> <li>→ Screening and approving data that is accessed and used by data owner or a convening organisation.</li> <li>→ Perhaps need additional peer review by experts to ensure that data is trusted.</li> </ul>			But no-one model has access to all the data
<p>WHO?</p> <p>Stakeholders across industry, academia and government</p>				
<p>HOW?</p> <p>Size of the funding required</p> <p>Skills, partnerships and structures</p>	<ul style="list-style-type: none"> <li>→ Training, skills &amp; awareness</li> <li>→ Developing skills in IP, trade secrets, cybersecurity, digital trust, and data governance across academia, industry, and supply chains.</li> <li>→ Publicly funded experts to guide SMEs and/or pilots</li> </ul>			





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