The Impact of Digitalisation on Science: Workflows, Outputs, and Trust

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The digital transformation of science is reshaping not only research workflows but also the integrity, openness, and societal trust in scientific knowledge. This paper investigates these developments through the lens of the Leibniz ScienceCampus DiTraRe and its interdisciplinary work on digital research infrastructures. Tracing the historical foundations of digital science – from Leibniz's binary logic to the AI-driven research environments of today – we highlight how shifts in data collection, knowledge organisation, and publication cultures redefine what constitutes scientific evidence and reproducibility.

We examine contemporary challenges and potentials through the use case of the Chemotion Electronic Lab Notebook, demonstrating how domain-specific digital tools can foster transparency, efficiency, and trustworthiness across research lifecycles. A particular focus is placed on the role of artificial intelligence (AI), including generative models and large language models (LLMs), which are increasingly integrated into scientific processes. We discuss emerging practices such as multi-agent LLM collaboration to mitigate hallucinations and the rise of autonomous AI research assistants like Sakana AI's "AI Scientist".

At the same time, the paper addresses the ethical and epistemic challenges posed by algorithmic processes, the impact of digitalisation on public trust, and the institutional responses through guidelines from DFG, UNESCO, and the European Commission. By connecting technical developments with cultural and normative reflections, we argue that building trusted digital research workflows requires a careful balance between innovation and responsibility, supported by interdisciplinary collaboration and continuous governance.

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1 Introduction

The Science Campus DiTraRe[1] investigates the digital transformation of research, focusing on how scientific workflows and research outputs have already evolved – and will continue to change – through digitalisation, and what this means for trust in science. DiTraRe examines the effects and potentials of digitalisation in areas such as data collection, knowledge organisation, the use of artificial intelligence (AI), handling of sensitive data, and changing publication cultures.

Research clusters address specific use cases, while cross-cutting dimensions explore overarching issues. This contribution highlights two of these dimensions – Reflections & Resonance and Tools & Processes – alongside the research cluster Smart Data Acquisition, using the "Chemotion Electronic Lab Notebook" as a use case to examine current challenges and opportunities in the digitalisation of science, particularly in light of recent developments in AI.

The article is structured as follows: Chapter 2 outlines a brief history of digitalisation in science. Chapter 3 discusses current AI-related challenges in science, with a focus on public trust and research integrity. Chapter 4 presents the "Smart Labs and AI" use case, exploring the digital transformation of research data practices. The conclusion summarises key developments, highlighting opportunities, challenges, and risks posed by AI in research.

2 History of digitalisation in science

The digitalisation of science is a multi-century journey that, in the context of the DiTraRe framework, is understood not only as a technological progression but also as a transformation of research infrastructures, knowledge practices, and the ways scientific trust and transparency are maintained. It has transformed how knowledge is generated, disseminated, and preserved. From early mechanical innovations to the rise of AI, each phase reflects evolving paradigms in research, communication, and epistemology. Today, with

1 The DiTraRe project, funded by the Leibniz Association and carried out by FIZ Karlsruhe and the Karlsruhe Institute of Technology from 2023 to 2027 (https://www.ditrare.de; *Visited on June 10, 2025*) deals with the influence of digital processes on research the influence of digital processes on research results, both in terms of research methods and in terms of with regard to communication in science and society.

the emergence of interdisciplinary initiatives such as the DiTraRe, this historical evolution is examined through the lens of changing research workflows, research infrastructure, scientific outputs, and the public's trust in science.

2.1 Foundations in Logic and Mechanisation (17th – 19th Century)

The roots of digital science can be traced to the work of Gottfried Wilhelm Leibniz, who introduced the binary number system in his 1703 publication *Explication de l'Arithmétique Binaire* and demonstrated how all numbers could be represented using only the digits 0 and 1 (O'Regan 2021). He also designed a logical calculating machine and envisioned a universal language of logic, which he termed the *calculus ratiocinator*, aiming to formalise human reasoning through symbolic logic (O'Regan 2021).

Born in 1646, Leibniz was not only a mathematician and inventor but also a philosopher who believed that human reasoning could be formalised through symbolic logic. His vision of the *calculus ratiocinator* aimed to express all rational thought in a formal language, anticipating later developments in computation and artificial intelligence (Smith 2007; O'Regan 2021). In this sense, the origins of AI lie not (only) in engineering but in a philosophical project concerned with modelling the structure of human cognition. This conceptual leap laid the groundwork for digital computation.

The 19th century saw further developments with Charles Babbage's Analytical Engine and Ada Lovelace, who is credited with writing the first algorithm, foreseeing a machine capable of manipulating symbols beyond arithmetic (Toole 1998). Meanwhile, Joseph Marie Jacquard's programmable loom (1801) demonstrated early mechanisation of control via punch cards.

2.2 Mathematical Formalism and the Birth of Computing (20th Century)

In 1936, Alan Turing formalised the concept of computation with the Turing machine, introducing a theoretical model of algorithmic processing in his seminal paper *On Computable Numbers, with an Application to the Entscheidungsproblem* (Turing 1936). Turing's work was deeply influenced by foundational developments in mathematical logic, particularly Kurt Gödel's incompleteness theorems (Gödel 1931), which had revealed the inherent limitations of formal axiomatic systems and intensified interest in the mechanisation of reasoning (Davis 2000). This line of thought also paralleled Alonzo Church's formulation of the lambda calculus, which arrived at equivalent conclusions concerning the limits of computation (Church 1936).

Around the same time, Claude Shannon's 1937 master's thesis applied Boolean algebra to switching circuits, laying the groundwork for digital logic – a theoretical insight that would later underpin modern digital circuit design (Shannon 1937, 1948). Together, these developments converged to establish the logical and physical basis of computing machinery, bridging abstract logic and engineering (O'Regan 2021; Ceruzzi 2000).

During World War II, programmable computers emerged, notably *Konrad Zuse's Z3* (1941), regarded as the first fully operational digital computer implementing binary arithmetic and programmability (Ceruzzi 2000; Randell 1973). A foundational advance followed with John von Neumann's *First Draft of a Report on the EDVAC* (1945), which introduced the concept of a *stored-program architecture*, where instructions and data share the same memory space – setting the standard for future computer systems (Neumann 1945; O'Regan 2021).

Networking and Personal Computing (1960s–1980s)

The ARPANET[2] project, initiated in 1969, connected multiple research institutions and later evolved into the modern Internet (Hafner and Lyon 1996). Meanwhile, the development of personal computers (e.g., Altair 8800, Apple I) in the 1970s began democratising computational access.

Digital tools found increasing application in research from the 1970s onward, notably in *early computational biology*, such as the first successful DNA sequencing efforts by Sanger and colleagues (Sanger, Nicklen, and Coulson 1977). At the same time, *expert systems* emerged in the field of artificial intelligence, enabling symbolic reasoning within narrowly defined domains – for example, MYCIN in medical diagnosis – marking a shift toward knowledge-based systems (Feigenbaum 1983; Buchanan and Shortliffe 1984). These developments laid the groundwork for rethinking how scientific data is collected, structured, and validated – an enduring concern for initiatives like *DiTraRe*, which interrogate the evolving dynamics of research in the digital age.

The World Wide Web and Open Science (1990s–2000s)

The launch of the World Wide Web by Tim Berners-Lee fundamentally transformed scientific communication and laid the groundwork for the development of integrated research

2 ARPANET stands for 'Advanced Research Projects Agency Network'. It was developed by the Advanced Research Projects Agency (ARPA) of the U.S. Department of Defense in the late 1960s and is widely considered the precursor to the modern internet. ARPANET was the first network to implement the TCP/IP protocol suite, and it enabled multiple computers to communicate on a single network – a revolutionary concept at the time.

infrastructures – such as those examined in DiTraRe – that enable new forms of collaboration, data sharing, and openness within the scientific community (Berners-Lee and Fischetti 1999). The emergence of online repositories like *arXiv.org*, which pioneered the open-access dissemination of preprints in physics and related fields (Ginsparg 1994), and open knowledge platforms such as *Wikipedia*, which crowdsources encyclopaedic content from global contributors (Lih 2009), further accelerated the global spread of information.

The digitisation of libraries – such as Google Books and the Internet Archive – and the rise of open access publishing have redefined how scientific texts are preserved, discovered, and accessed (Borgman 2007; Kahle 2007; Suber 2012). This shift has been accompanied by growing emphasis on data curation, metadata standards, and transparency in scientific outputs, as reflected in initiatives like the FAIR principles (Wilkinson et al. 2016). These are all central themes in DiTraRe's analysis of digital research workflows and infrastructure development.

2.3 Data-Driven Research and the AI Revolution (2000s–present)

The 21st century has seen a fundamental shift towards data-intensive science, actively explored by initiatives such as DiTraRe (Toole 1998). These initiatives examine both the technical and ethical dimensions of digital research workflows, focusing on how they can improve research quality and public trust. This shift has been driven by advances in cloud computing, big data infrastructures, and reproducibility tools such as Electronic Lab Notebooks (ELNs Toole 1998).

Large-scale projects like CERN's Large Hadron Collider illustrate the enormous scale of data modern science must handle (Evans and Bryant 2008; Bejar Alonso et al. 2020). Jim Gray's "The Fourth Paradigm" (2011) captured this transition, describing a new model of discovery where data exploration complements hypothesis-driven research.

AI and machine learning have since become integral to scientific workflows, reshaping how data is processed, interpreted, and applied across disciplines (Jordan and Mitchell 2015). Within DiTraRe, AI is applied to areas such as semantic data enrichment, metadata curation, automated annotation of research outputs, and predictive modelling (Jordan and Mitchell 2015). Through the use of Large language models like GPT-4 now practices in science are being reshaped with regard to knowledge processing and communication.

Emerging AI research assistants – such as Sakana AI's "AI Scientist" – are pushing the boundaries of autonomous scientific work. According to its creators, this system can generate novel research ideas, write and execute code, conduct simulations, summarise results, and even draft scientific manuscripts, complete with automated peer review to assess the quality of generated research content (Sakana AI 2024).

In addition, platforms like Elicit, SciSpace, and ResearchRabbit support researchers in literature discovery and comprehension. These tools use large language models to filter relevant publications, summarise complex findings, and visualise citation networks, thereby improving access to and understanding of scientific knowledge (Academia Insider 2024; Elephas 2024).

To address the persistent issue of AI hallucinations, researchers have begun experimenting with multi-agent collaboration techniques. In such frameworks, multiple LLMs are used to evaluate and cross-check each other's outputs, identifying errors and inconsistencies. Key techniques include:

- Adversarial debates, where models challenge one another's responses to promote consensus or correction (Yang et al. 2025),
- Uncertainty-Aware Fusion, which integrates outputs based on model confidence to reduce hallucinated content (Dey, Merugu, and Kaveri 2025), and
- Ensemble models with shared weights, which optimise resource use while improving output reliability (Arteaga, Schön, and Pielawski 2024).

These developments are not merely technical optimisations – they are essential steps toward building trustworthy AI systems in scientific contexts.

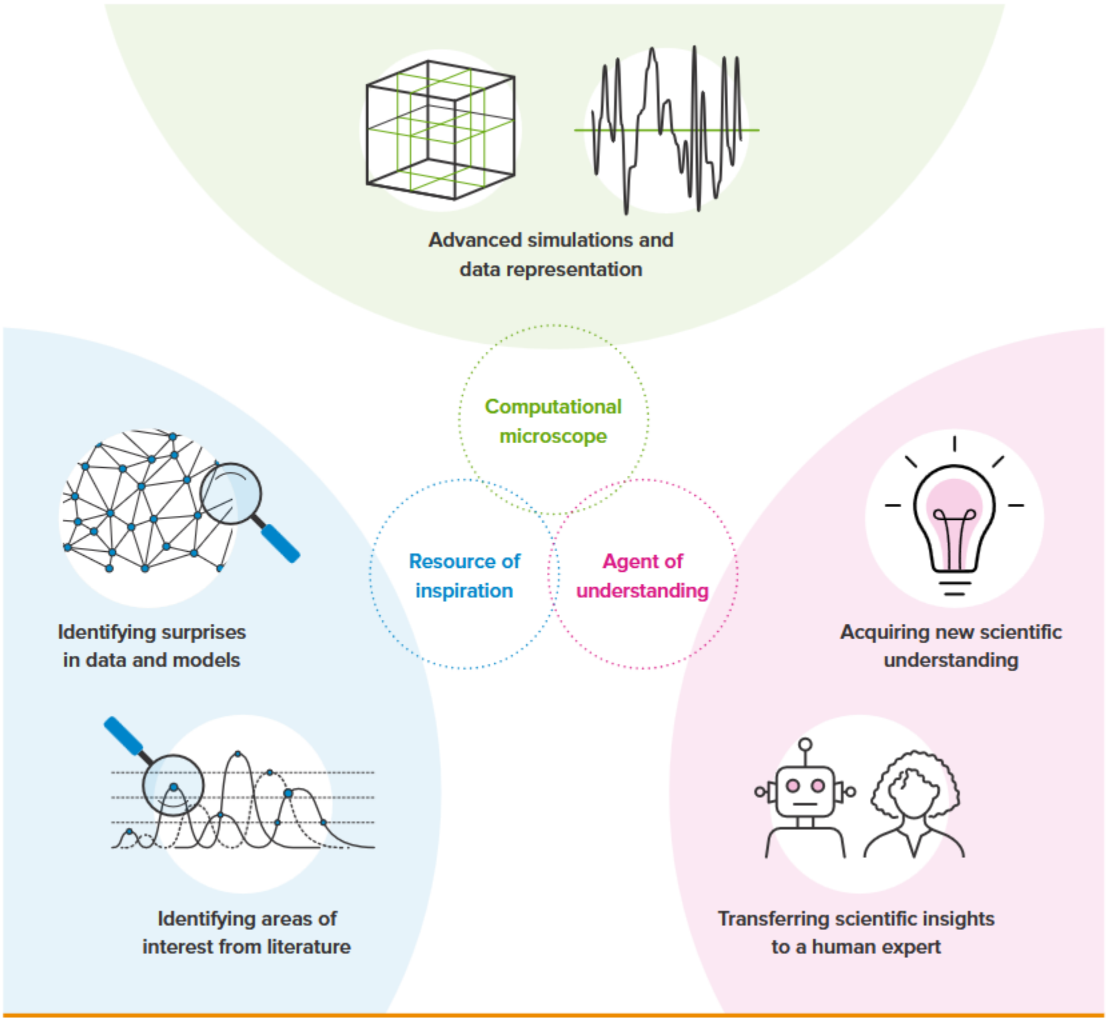
The DiTraRe initiative actively engages with these advances, assessing both their transformative potential and associated risks. Of particular interest are questions of research integrity, transparency, and public trust in a time when AI is increasingly involved in producing and interpreting scientific knowledge.

According to the Royal Society, AI can support scientific understanding in three key ways (The Royal Society 2024, p. 31), shown in Figure 1:

- Computational Microscope: Simulating and visualising data in ways experiments alone cannot.
- Resource of Inspiration: Providing novel, unexpected insights.
- Agent of Understanding: In theory, autonomously generating and communicating knowledge – though this remains a conceptual frontier.

While AI has shown surprising capabilities, it has not yet reached true autonomy in understanding.

Reproduction of a visualisation of the three general roles of AI for scientific research as either a computational microscope, resource of human inspiration, or an agent of understanding[124].



124 The diagram describes three possible ways in which AI can contribute to scientific understanding. The 'computational microscope' refers to the role of AI in providing information through advanced simulation and data representation that cannot be obtained through experimentation. 'Resource of inspiration' refers to scenarios in which AI provides information that expands the scope of human imagination or creativity. The 'agent of understanding' illustrates a scenario in which autonomous AI systems can share insights with human experts by translating observations into new knowledge. As of yet, there is no evidence to suggest that computers can act as true agents of scientific understanding. See: Krenn M. *et al.* 2022. On Scientific Understanding with Artificial Intelligence.

Figure 1: Three possibilities for AI supported scientific understanding (Source: The Royal Society 2024, p. 31).

Generative AI promises increased efficiency in idea generation, literature review, and writing (Albrecht 2023), but it also raises challenges around transparency, bias, and authorship (Fecher et al. 2023; Messeri and Crockett 2024). Multi-model strategies represent one way forward, ensuring that AI becomes not just faster, but also more reliable and responsible in supporting scientific work.

3 AI in science: public trust & research integrity

In light of AI, the digitalisation of research affects not only how science is conducted but also how it is perceived by the public. Factors such as transparency, data openness, and the potential for reproducibility can enhance public trust in scientific processes (Elliott 2017; Floridi and Cowls 2019). However, looking towards AI, the reliance on black-box AI systems and large-scale datasets raises concerns about the reliability and accessibility of scientific findings. Especially as recent development in generative AI challenges workflows, infrastructures and outputs in science (Schreiber and Ohly 2024). On the one hand, generative AI provides new chances for knowledge generation and processing, e.g. by an increased efficiency and productivity in scientific working practices with various possible applications. It further provides potentials for research data, since it offers potentials in training small data sets, and enables LLM-based knowledge extraction from data bases and provides easier programming tools (Digital Science et al. 2023). On the other hand, there are many open questions related to generative AI in science. These range from technical limits and touch the transparency and traceability of scientific results with regard to detection, authentication and the widely cited "hallucinations" (European Research Council 2023). With regard to competences and skills, AI-literacy of researchers comes into play. Further ethical questions of the use of generative AI come up and aspects like overreliance, spread of false information, biased knowledge or source misrepresentation (Jahnel et al. 2025).

The digitalisation of research not only affects how science is conducted but also how it is perceived by the public.

Focusing on generative AI and open data, challenges on two levels come up with regard to trust in science: (1) trust in science from the public as well as (2) research integrity within science. While in general, trust in science remains high, there are four components of trust in scientists which encompass competence, integrity, benevolence and openness (Cologna et al. 2025, p. 714). The components are defined (Mede and Cologna 2025): Competence encompasses the expertise, intelligence, and qualifications required to conduct high-quality research. Integrity is about how honest, ethical, and sincere scientists are. Benevolence addresses how much scientists care about the well-being of others, improving the lives of others, and considering the interests of others. Openness asks how open scientists are to feedback, transparency, and consideration for the view of others. When looking at generative AI, the aspect of integrity as well as openness are of particular interest – while recent developments in the use of generative AI in science may challenge research integrity due to epistemic risks and also other types of misuse, e.g., plagiarism, cheating, generate fictitious data and analyses (Meça and Shkëlzeni 2023). According to Cologna et al. the openness aspect is currently more challenging, since the public perception of the openness of scientific practices is lower than the perceived trust in research integrity. With respect to research data management practices to keep research integrity high are touched in this article. However, there could be further attempts to increase the public perception of openness in science, e.g., by more communication of results to the public (see Figure 2, Cologna et al. 2025, p. 719). Measures proposed embrace being receptive to feedback, transparent about funding and data sources, communicating about science with the public by encouraging public participation in genuine dialogue, including insights and needs of societal actors.

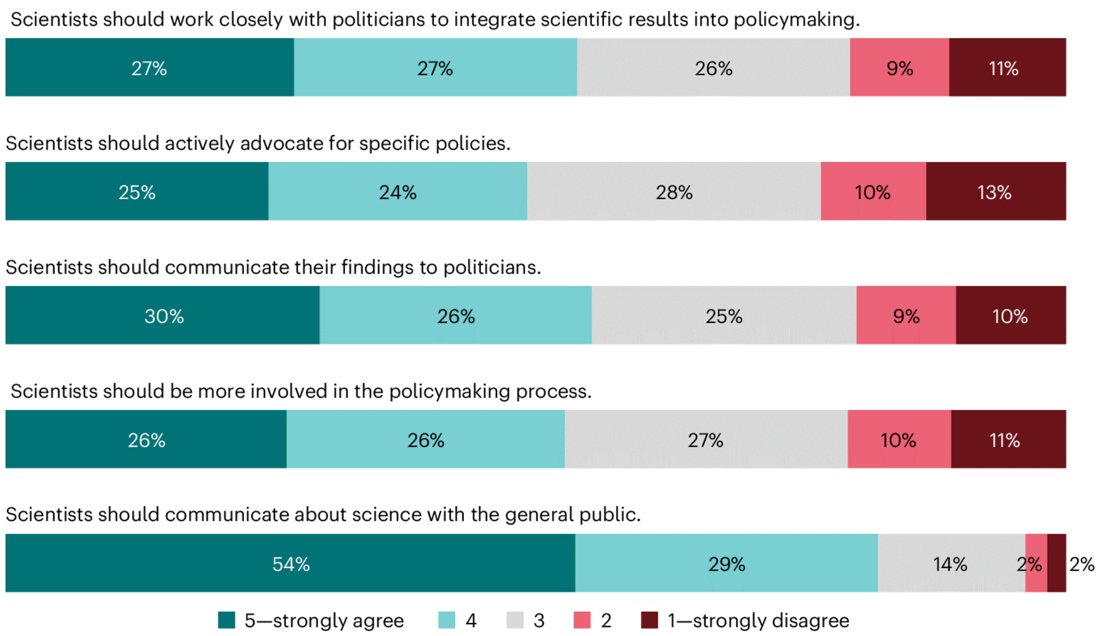


Figure 2: Normative perception of scientists in society and policy making (Cologna et al. 2025).

Open science and open data have traditionally been seen as key to building public trust, as highlighted by Rosman et al. (2022). In their study, participants were asked about the importance of open science practices and whether scientists who adopt these approaches are perceived as more trustworthy. The vast majority considered it important for researchers to make their findings publicly accessible and to follow open science principles. Most participants also reported greater trust in science when materials, data, and code were openly available.

To further strengthen public trust in open data, especially when using AI, several measures can be taken. First, ensuring the reproducibility of AI-based research is essential. This can be supported through reproducibility checklists, standardized data-sharing protocols, and field-specific reproducibility guidelines. Additionally, investing in open repositories is critical. This includes the sharing of datasets, software versions, and workflows, as well as developing context-aware documentation to help adapt AI models to local research settings (The Royal Society 2024, p. 13). Albeit these measures, still modes of engaging and communicating with the public have to developed and explored for the specific context of open data research and practice.

Moreover, in the upcoming use of generative AI in science there might be the risk that research integrity erodes, thus science-internal quality assurance needs to be built up in order to remain high. Up to now, there are several guidelines and statements published with regard to the use of generative AI in science. One widely cited statement is that of the German Research Association (Deutsche Forschungsgemeinschaft 2023). In this statement, the use of generative AI is supported, but binds to the principles of good scientific practice and the transparency and traceability of scientific results. However, the use of models should be thoroughly disclosed and a discursive process including experiences with generative AI is envisaged (Deutsche Forschungsgemeinschaft 2023). Other guidelines focus on the importance of the human factor, "[...] the usage processes should ensure humans' interactive engagement with GenAI and higher-order thinking, as well as human accountability for decisions related to the accuracy of AI-generated content, and their impact on human behaviours" (UNESCO 2023, p. 29) or point out the communicative process of all actors of the science system: "[...] publishers and researchers at all stages of their careers are essential in shaping the discussion on AI and how it can serve the public interest in research" (European Commission 2024, p. 4).

4 Creating Trusted Digital Research Workflows: A Cultural Challenge

The digitalisation of research is transforming not only the tools we use but also the way scientific knowledge is generated, validated, and shared. This transformation, however, is not purely technological – it is profoundly cultural (OECD 2020). In this chapter, we examine how trusted digital research workflows can be developed and sustained. We focus in particular on laboratory practices in chemistry, drawing on insights from the DiTraRe use case *Smart Data Acquisition* and the Electronic Lab Notebook (ELN) *Chemotion*[3]. Through this lens, we explore how digital infrastructures influence everyday scientific work, the nature of research outputs, and the reproducibility of experimental results.

4.1 From Infrastructure to Cultural Practice

The digitalisation of research entails more than the integration of new technologies or software platforms; it necessitates a fundamental transformation of the epistemic cultures that define individual scientific disciplines. These cultures have evolved over time through established methodologies, procedural routines, and disciplinary tools. Each field possesses distinct norms regarding what constitutes valid evidence, how experiments are conducted and recorded, and the frameworks through which data are interpreted. Such

3 http://www.chemotion.net; *Visited on June 10, 2025.*

entrenched disciplinary practices play a critical role in shaping both the adoption and perceived credibility of digital workflows. This influence is clearly illustrated in the field of chemistry, as demonstrated in Figure 3 which compares a laboratory notebook from 1927 with one from today (Herres-Pawlis, Liermann, and Koepler 2020). Despite a century of technological advancement, experimental documentation is still predominantly conducted with pen and paper (Butler 2005). This persistence of analogue practices highlights the extent to which digitalisation in science is entangled with cultural inertia.

Meanwhile, as described in Chapter 2, the evolution of computing technologies has led to powerful tools that enable standardised, computer-assisted workflows. These workflows hold enormous potential to enhance the reliability, efficiency, and reproducibility of research. Yet their implementation remains uneven, and their success depends as much on social acceptance and institutional support as on technical innovation (National Academies of Sciences, Engineering, and Medicine 2022).

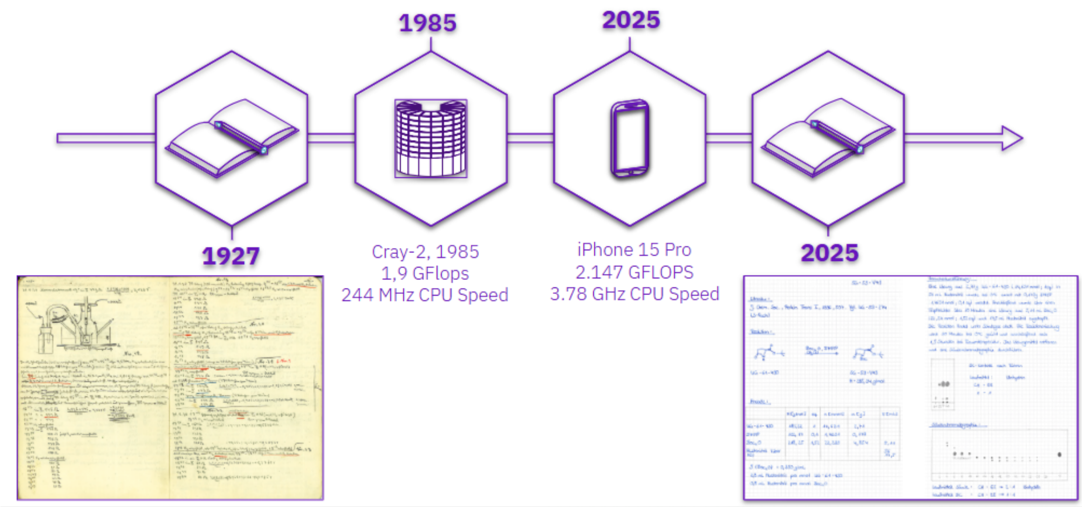


Figure 3: Comparison of the evolution of laboratory notebooks and computers: Despite decades of digitalisation, traditional paper lab notebooks remain widespread (Herres-Pawlis, Liermann, and Koepler 2020).

4.2 Creating Trustworthy Digital Workflows

The question, then, is not simply how to digitalise, but how to do so in a way that researchers can trust and adopt. Initiatives such as NFDI4Chem[4] provide important answers. They demonstrate how digital workflows can support researchers across the entire data life cycle – spanning data acquisition, processing, analysis, publication, and long-term preservation – by adhering to open, interoperable standards.

4 Chemistry Consortium in the National Research Data Infrastructure – http://www.nfdi4chem.de; *Visited on June 10, 2025.*

Central to this approach is the development of user-friendly, domain-specific tools such as Chemotion ELN. Designed specifically for the needs of chemists, Chemotion ELN enables structured and semantically rich documentation of experimental data, helping ensure both interpretability and reproducibility. Rather than replacing researchers' practices, it extends them into digital spaces where data can be preserved, shared, and reused.

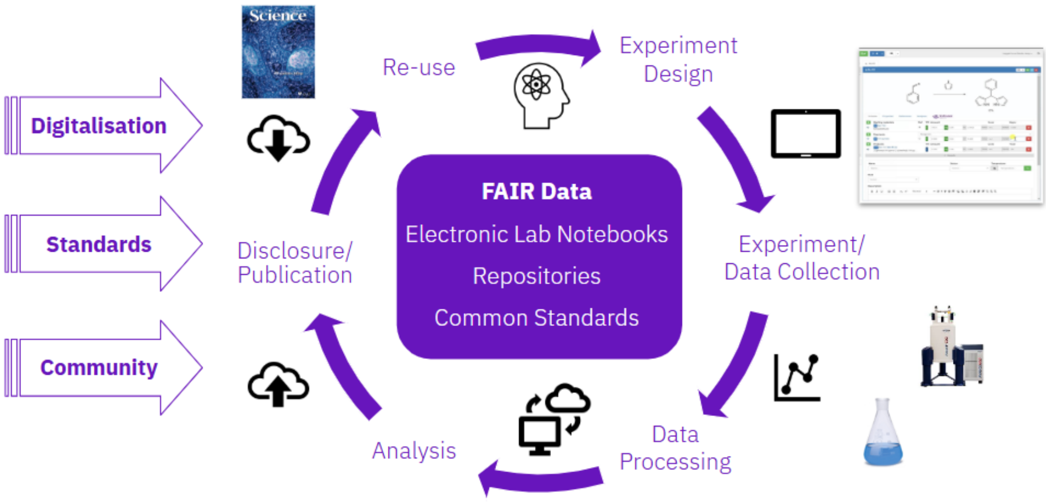


Figure 4: From analogue to FAIR: Digital workflows in chemistry as proposed by NFDI4Chem using Chemotion ELN and FAIR data repositories like RADAR4Chem (Source: NFDI4Chem).

With tools like Chemotion, chemists can record structured data in a semantically rich way, ensuring interpretability and reproducibility. The resulting FAIR data can then be stored in repositories like RADAR4Chem[5], guaranteeing long-term access and global reusability – fuelling a new cycle of data-driven science.

4.3 Chemotion: A Model for Trusted Research Digitalisation

The Chemotion platform exemplifies a comprehensive and integrated approach to digitalisation in the chemistry laboratory. It enables researchers to document experimental workflows, chemical reactions, and results in a structured, machine-readable format. This not only facilitates the systematic organisation of data but also substantially improves reproducibility by reducing the risk of human error and ensuring that experimental conditions are recorded with precision.

Standardisation plays a key role in Chemotion's design. By using consistent data formats and controlled vocabularies, the platform ensures compatibility with other digital research

5 https://radar4chem.radar-service.eu/radar/en/home; *Visited on June 10, 2025.*

tools and repositories, thereby supporting interoperability across systems and institutions. In practice, this means that data entered into Chemotion can be seamlessly exported, analysed, or shared – forming a coherent link in a broader digital research infrastructure.

Another important feature is the automation of data logging. Chemotion can directly capture outputs from laboratory instruments, streamlining the recording process and reducing the administrative burden on researchers. This automation also enhances data accuracy and consistency, since manual transcription steps – where errors frequently occur – are minimised.

Crucially, Chemotion supports collaborative work through cloud-based access. Researchers from different institutions or disciplines can work together in shared digital environments, enabling more efficient knowledge exchange and interdisciplinary experimentation. The platform's design is also aligned with the FAIR principles – ensuring that data is findable, accessible, interoperable, and reusable. This is particularly important for promoting sustainable open science, where datasets remain usable and meaningful over time.

From a compliance perspective, Chemotion offers tangible benefits as well. Its structured documentation makes it easier to fulfil regulatory and laboratory safety requirements (Tremouilhac et al. 2020). The ability to track, search, and verify digital records simplifies audit processes and helps demonstrate adherence to standards of good scientific practice. In sum, Chemotion represents a major step forward in the digitalisation of laboratory research – enhancing not only efficiency and reproducibility, but also transparency and trust.

4.4 Beyond Digitalisation: The Role of AI in Research Workflows

As digital infrastructures mature, AI is becoming an increasingly important actor in shaping how data is curated, interpreted, and reused. Within platforms such as ELN and research data repositories, AI technologies have the potential to augment laboratory workflows in numerous ways. In DiTraRe, we have identified several promising measures in this regard, that are described in the following and that we plan to implement and evaluate during the project.

One of the most immediate benefits lies from our perspective in the automatic extraction and standardisation of metadata. AI systems can analyse raw experimental data and generate relevant metadata entries, reducing the amount of manual input required and improving consistency across records. In tandem, machine learning models can classify and tag chemical reactions or compounds based on their content and contextual relationships, facilitating more efficient data management.

AI also enhances data integrity through predictive data cleaning and anomaly detection, as we believe. By identifying inconsistencies or missing information within datasets, it supports higher standards of data quality. Natural Language Processing (NLP) techniques extend these capabilities further by integrating information from research literature and patents, linking experimental data with existing knowledge and enhancing the contextual understanding of results.

The creation of chemistry-specific knowledge graphs through semantic analysis allows for more intuitive data discovery, helping researchers navigate complex data landscapes and uncover new relationships between concepts, substances, and reactions. AI can also support experimental design by analysing prior reaction data and recommending optimised conditions, thereby reducing reliance on trial-and-error methods.

On the user interface level, AI-powered search functions enable context-aware querying of experimental data, making it easier for researchers to locate relevant datasets or protocols. Finally, AI can assist in summarising results and generating structured reports, offering insights that might otherwise remain hidden in the data.

From our perspective, these capabilities mark a significant shift in how research is conducted and interpreted. AI moves from being a back-end tool to a semi-autonomous partner in the scientific process, suggesting hypotheses, identifying trends, and enabling new modes of data-driven discovery.

4.5 Reflection on the Use Case

Also, with respect to open data, generative AI has the potential to strengthen and transform open research data. It can improve small datasets and metadata quality, but can also bring interactive elements, e.g. by acting as a virtual collaborator (Digital Science et al. 2023).

It seems that also for open research data, new forms of Human-AI-Collaboration might emerge. However, this requires clearly defining the role of human verification in research. But how much should AI handle, and where do we draw the line for human verification? And given the pure amount of data sets, where are the limits of “human-in-the-loop” approaches?

This shift also changes how we organise competences in the field of open research data, since competences and skills change and a specific AI literacy is needed, or in other words, there is a change from human control knowledge to translational knowledge (National Academies of Sciences, Engineering, and Medicine 2022).

In order to govern this change, standards and guidelines are needed. Challenges include the rapid pace of AI developments, which often outstrip the ability of guidelines to keep up with emerging functionalities and applications. On the other hand, the development and implementation of the guidelines raises questions of responsibility. Should research communities lead the way, or should top-down regulations set the framework? And how can a discursive process between the two levels be organised? And lastly, how detailed should guidelines be to remain practical? In order to follow a smooth implementation for a scalable and effective AI integration in research, these key questions have to be tackled by the open data community in a joint approach, also including relevant actors of the science system.

5 Conclusion

The digital transformation of science reaches far beyond the mere adoption of new technologies. As we have shown throughout this contribution, it reshapes fundamental aspects of how research is conducted, how results are documented and shared, and how trust in scientific knowledge is created and maintained – both within science and in its relation to society.

At the heart of this transformation is a cultural challenge. While the technical means for digitalisation are often available, their integration into established scientific workflows requires a shift in epistemic practices and disciplinary habits (The Royal Society 2024). Our exploration of laboratory work in chemistry, through the DiTraRe use case Smart Data Acquisition and the Electronic Lab Notebook Chemotion, has highlighted this vividly: despite a century of technological advancement, paper-based documentation remains widespread, signalling the persistence of analogue routines.

However, tools like Chemotion illustrate how digital infrastructures – if designed in alignment with domain-specific needs – can enable not only standardisation and reproducibility but also a more collaborative and transparent research process. By facilitating FAIR data practices and integrating structured workflows, Chemotion supports both scientific integrity and open science. When combined with repositories such as RADAR4Chem[6] and other repositories for chemistry data recommended by NFDI4Chem[7], it contributes to a sustainable cycle of data-driven discovery.

The inclusion of AI adds a new dimension to this development. AI can assist with metadata curation, semantic annotation, error detection, and even hypothesis generation (Digital Science et al. 2023). These capabilities point toward a shift from manual documentation to machine-augmented understanding. Yet, this shift also raises new questions:

6 https://radar4chem.radar-service.eu/; *Visited on June 10, 2025.*
7 https://www.nfdi4chem.de/repos/; *Visited on June 10, 2025.*

What remains the role of human oversight? How transparent are the processes behind AI-generated outputs? And what standards must be in place to ensure that AI contributes to, rather than undermines, the integrity of research?

These questions also extend to public trust. On the one hand, we argue that the principles of open science – transparency, reproducibility, accessibility – are strengthened through digitalisation and AI. On the other hand, reliance on algorithms and vast datasets can alienate non-specialist audiences and challenge the transparency and integrity of the scientific process (European Research Council 2023). As survey data shows, trust in scientists is generally high, but it is conditional on perceived openness, competence, and accountability. Maintaining and enhancing that trust requires not only technical solutions but also deliberate strategies in science communication and governance. To address these issues, institutional frameworks must keep pace with technological innovation (Cologna et al. 2025). National and international bodies – such as Deutsche Forschungsgemeinschaft (2023), UNESCO (2023), and the European Commission (2024) – are beginning to articulate principles and recommendations for the responsible use of generative AI in research. These efforts are essential, but they must be complemented by bottom-up initiatives within research communities, where disciplinary standards, peer review practices, and ethical guidelines are continuously developed and discussed.

Ultimately, trusted digital research workflows emerge at the intersection of technical infrastructure, cultural change, and institutional reflection. They are not simply adopted; they are cultivated (Jacyszyn et al. 2025). The DiTraRe initiative contributes to this cultivation by fostering interdisciplinary dialogue and by developing exemplary use cases that demonstrate both the potential and the limitations of digitalisation in science.

As science enters the age of AI, we are witnessing not only new tools but new ways of knowledge generation and procession. This calls for shared responsibility of researchers as well as actors of the science system alike: to shape the future of research in a way that is open, transparent, and worthy of trust. Continued exchange and a dedicated guideline on the use of generative AI in research data management practice might be valuable start.

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Authorship Contributions

- Felix Bach: Conceptualisation; Methodology; Writing – Original Draft; Supervision; Data Curation; Review & Editing.
- Linda Nierling: Theoretical Framework; Writing – Original Draft; Writing – Review & Editing; Ethical Reflection; Integration of TA perspectives.
- Christian Bonatto Minella: Writing – Review & Editing; Interoperability Aspects; Proofreading.
- Angelina Sophie Dähms: Writing – Review & Editing, Literature Review; Proofreading.

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