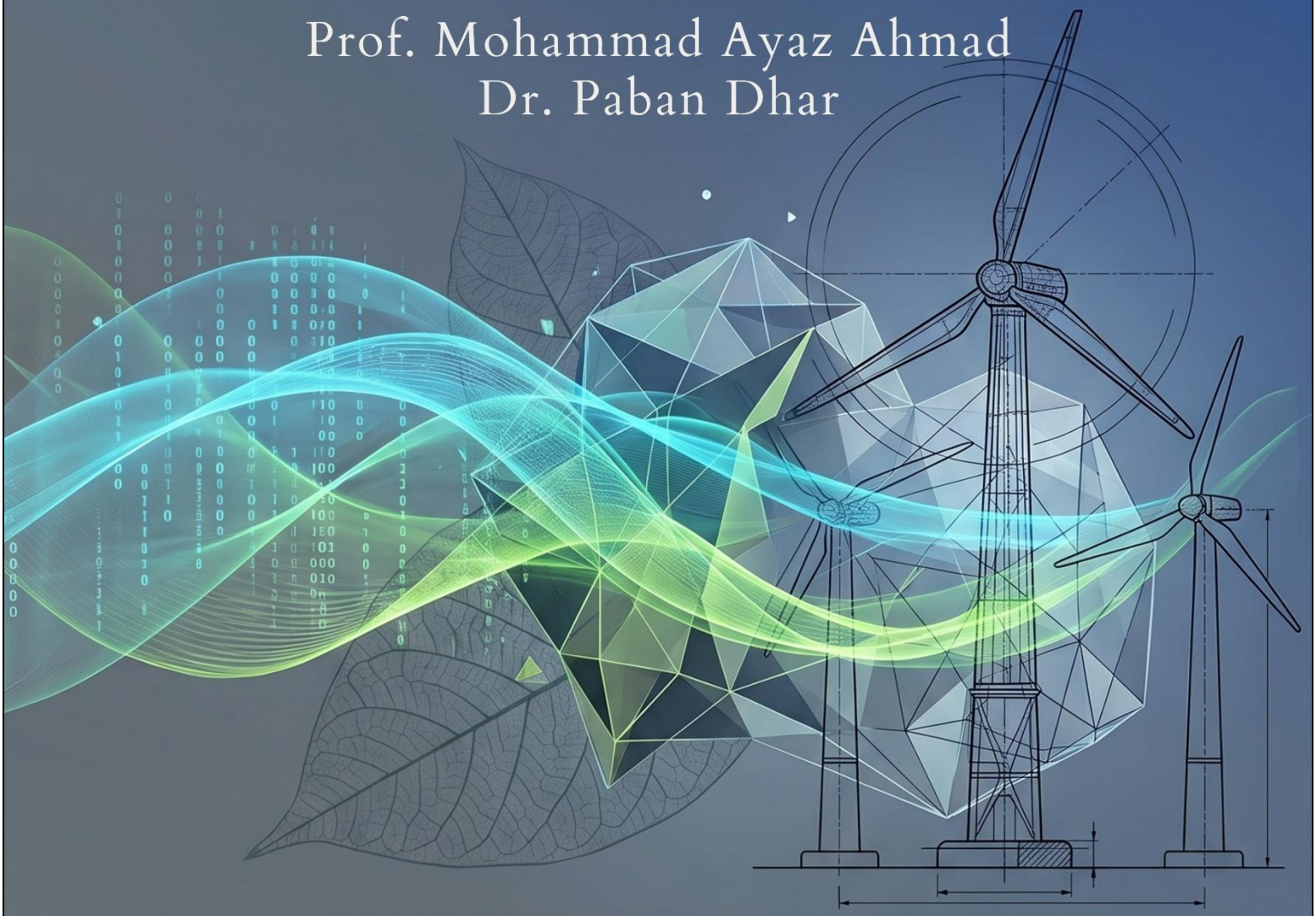
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Progress in Science and Engineering Research: Trends and Real-World Solutions

Editors:
Dr. Madhulika Dutta
Dr. Shahnaz Kossar
Prof. Mohammad Ayaz Ahmad
Dr. Paban Dhar



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PREFACE

Science and engineering are fundamental drivers of innovation, economic growth, and societal progress. Continuous advancements in scientific knowledge and engineering technologies are transforming industries, improving quality of life, and providing practical solutions to complex global challenges. *Progress in Science and Engineering Research: Trends and Real-World Solutions* highlights contemporary developments, emerging research directions, and innovative applications that connect theoretical understanding with practical implementation.

This volume explores diverse areas of science and engineering, emphasizing technological advancements, interdisciplinary collaboration, and evidence-based approaches to problem-solving. Developments in materials science, artificial intelligence, computational technologies, biotechnology, environmental science, energy systems, electronics, and engineering design are creating new opportunities for innovation. These advances contribute to improved industrial processes, sustainable infrastructure, efficient resource utilization, environmental protection, and the development of reliable technological solutions.

A significant focus of modern research is translating scientific discoveries into applications that address real-world needs. Innovative methodologies, experimental investigations, digital tools, and advanced analytical techniques enable researchers to develop effective responses to challenges in healthcare, manufacturing, agriculture, transportation, energy, and environmental management. The integration of scientific principles with engineering practices further strengthens technological efficiency, promotes sustainable development, and supports informed decision-making. Responsible innovation, research integrity, safety, and environmental considerations remain essential for ensuring meaningful and lasting progress.

The book is intended for researchers, academicians, engineers, scientists, students, and professionals seeking insights into contemporary scientific and technological developments. By presenting diverse perspectives and practical applications, it encourages interdisciplinary learning, collaborative research, and the exploration of emerging opportunities.

It is hoped that this volume will serve as a valuable academic resource and inspire further investigation, creative thinking, and technological advancement. By emphasizing research and practical solutions, this book bridges science, engineering, and society to foster a sustainable, technologically advanced future.

- Editors

TABLE OF CONTENT

Sr. No.	Book Chapter and Author(s)	Page No.
1.	**EMERGING RESEARCH PARADIGMS IN MODERN SCIENCE AND TECHNOLOGY** Vivek Kumar and Sorabh	1 – 11
2.	**ARTIFICIAL INTELLIGENCE AND DIGITAL TWINS FOR PREDICTIVE MAINTENANCE OF AEROSPACE SYSTEMS** Vijayakumar P and Karthik M	12 – 25
3.	**DATA-DRIVEN ARTIFICIAL INTELLIGENCE METHODS, APPLICATIONS AND FUTURE PERSPECTIVES** Vivek Kumar and Sorabh	26 – 35
4.	**TURNING CO_2 INTO VALUABLE CHEMICALS: THE CHEMISTRY AND TECHNOLOGY OF ELECTROCHEMICAL CARBON UTILIZATION** Mohammed Azam Shaikh	36 – 47
5.	**A SOLVENT-FREE, MICROWAVE-ASSISTED GREEN PROTOCOL FOR SYNTHESIZING 1,2-DISUBSTITUTED BENZIMIDAZOLES** Priyabrata Roy	48 – 57
6.	**AN ANALYTICAL STUDY OF CHAIN OF CUSTODY IN DF** Babli Kumari and Prabhat	58 – 70
7.	**ADVANCED FUNCTIONAL NANOMATERIALS: CHEMICAL DESIGN, CHARACTERIZATION AND REAL-WORLD APPLICATIONS** Divya Chenna	71 – 84
8.	**NANOPARTICLE: THE BEST VERSION OF CATALYST FOR THE SYNTHESIS OF THIAZOLE DERIVATIVES** Ashwini Narale, Shivam Gore, Dnyandev Bhosale and Anjana Lawand	85 – 99
9.	**GREEN CHEMISTRY: PRINCIPLES, PROGRESS, AND PROMISE** Divya Chenna	100 – 113
10.	**DELETERIOUS EFFECTS OF SMARTPHONE RADIATIONS ON THE REPRODUCTIVE HEALTH OF MALES: A MINI-REVIEW** Prakash Chandra Gupta	114 – 118

11.	**FROM BLACK-BOX MODELS TO TRANSPARENT DECISIONS: ADVANCES AND CHALLENGES IN EXPLAINABLE ARTIFICIAL INTELLIGENCE** Rupali Parihar and Pooja Rana	119 – 128
12.	**INTEGRATING TECHNOLOGICAL INNOVATION AND ADAPTIVE PATHWAYS TOWARD CLIMATE-SMART FOOD SYSTEMS** Eeda Bheem Mahendra Roy and Eeda Susrutha	129 – 133
13.	**REGENERATED CELLULOSE FOR FLEXIBLE AND GREEN ELECTRONICS** Kailash Nemade	134 – 140
14.	**FUNDAMENTAL PROPERTIES AND SYNTHESIS OF SILVER SULPHIDE THIN FILMS** Prashant A. Chate and Dattatray J. Sathe	141 – 149
15.	**BRIDGING DISCOVERY AND DEPLOYMENT: QUANTIFYING TRENDS, TECHNOLOGY READINESS AND REAL-WORLD SOLUTIONS IN SCIENCE AND ENGINEERING RESEARCH** Nenavath Madhu Sri	150 – 154

Progress in Science and Engineering Research: Trends and Real-World Solutions
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EMERGING RESEARCH PARADIGMS IN MODERN SCIENCE AND TECHNOLOGY

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Abstract

Science and technology research is undergoing significant changes due to the rapid development of artificial intelligence, machine learning, big data, biotechnology, advanced materials, robotics, quantum technologies, and sustainable technologies. These emerging paradigms are changing traditional approaches to scientific investigation by promoting computational analysis, automated experimentation, interdisciplinary collaboration, open science, and data-driven decision-making. They provide new opportunities for faster scientific discovery, improved technological innovation, advanced healthcare, industrial development, environmental management, and sustainable development. At the same time, their growing use creates challenges related to research reproducibility, data privacy, algorithmic bias, research integrity, intellectual property, unequal access to advanced infrastructure, and environmental costs. This chapter examines the evolution of research paradigms and discusses major emerging trends and methodologies shaping contemporary science and technology research. It further analyses their impact on scientific discovery, technological development, healthcare, industry, society, and environmental sustainability. Attention is also given to ethical considerations and the need for responsible governance. The chapter concludes that future research should combine technological innovation with transparency, human judgement, interdisciplinary collaboration, sustainability, and ethical responsibility. Such an approach can help ensure that emerging research paradigms contribute to reliable scientific knowledge, practical technological solutions, and broader societal benefits.

Keywords: Emerging Research Paradigms, Artificial Intelligence, Machine Learning, Big Data, Biotechnology, Research Innovation, Open Science, Sustainable Technology.

1. Introduction

Scientific and technological research is undergoing substantial changes as new tools, methods, and forms of collaboration reshape the way knowledge is produced and applied. Traditional research has largely relied on observation, experimentation, theoretical analysis, and discipline-specific approaches. These methods remain important, but many contemporary scientific and societal problems are complex and interconnected, requiring contributions from multiple areas of

knowledge and research expertise (OECD, 2015; UNESCO, 2021). Consequently, research is increasingly moving toward interdisciplinary, collaborative, and integrated approaches.

The rapid development of digital technologies has further transformed the research process. Artificial intelligence, machine learning, big data analytics, cloud computing, high-performance computing, advanced scientific instruments, and automated laboratory systems are increasingly being incorporated into research activities. These technologies allow researchers to manage large datasets, perform complex computational analyses, develop predictive models, and conduct experiments with greater speed and precision. The growing integration of computational and experimental approaches has therefore created new possibilities for scientific discovery and technological development (National Academies of Sciences, Engineering, and Medicine [NASEM], 2019).

Another important development is the increasing emphasis on open and collaborative research. The sharing of scientific publications, research data, methods, and other research outputs can improve transparency, accessibility, collaboration, and the potential for reproducibility (UNESCO, 2021; NASEM, 2019). At the same time, emerging technologies raise important concerns related to research integrity, data privacy, ethical responsibility, unequal access to research infrastructure, and the environmental costs of advanced computing.

This chapter examines the major emerging paradigms in science and technology research, with particular attention to current trends, changing research methodologies, technological developments, and their impacts on science, industry, society, and the environment. It also discusses important challenges and future directions for responsible, transparent, and sustainable scientific research.

2. Evolution of Research Paradigms

Scientific research has evolved considerably from relatively individual, discipline-specific investigations toward large-scale, collaborative, interdisciplinary, and technology-supported research. Earlier research practices were primarily based on direct observation, laboratory experimentation, theoretical reasoning, and manual analysis. These approaches established the foundations of modern science, but the increasing complexity of scientific questions has required researchers to combine knowledge, methods, and expertise from multiple disciplines. Contemporary research increasingly involves large teams, specialized facilities, international collaboration, and complex research infrastructures (National Academies of Sciences, Engineering, and Medicine [NASEM], 2019).

A major transition has been the movement from predominantly experimental research toward computational and data-intensive research. Advances in computing, digital instruments, databases, and statistical methods have made it possible to analyse very large and complex datasets. Computational modelling and simulation now complement laboratory and field

experiments, allowing researchers to investigate systems that may be difficult, expensive, or time-consuming to study directly. This has strengthened the connection between theoretical, experimental, and computational approaches.

Another important paradigm is interdisciplinary research, in which researchers from different scientific and technological fields work together to address problems that cannot be adequately solved within one discipline. Areas such as climate change, public health, biotechnology, artificial intelligence, energy, and environmental sustainability increasingly require such integrated approaches (OECD, 2015).

Research is also becoming more open and transparent. Sharing data, methods, software, and research outputs can improve verification, reproducibility, and collaboration. NASEM (2019) emphasized that transparent reporting and access to appropriate data and computational materials are important for strengthening confidence in scientific findings. Thus, modern research is increasingly characterized by collaboration, digital tools, data sharing, and integration of multiple methods rather than reliance on a single research approach.

3. Major Emerging Trends in Science and Technology Research

Science and technology research is increasingly shaped by rapid advances in digital systems, biotechnology, advanced materials, automation, and sustainable technologies. A major feature of current research is the convergence of previously separate fields. Artificial intelligence is being combined with biology, materials science, robotics, computing, and environmental research, while developments in quantum technologies and synthetic biology are creating new research possibilities. The OECD identifies artificial intelligence, synthetic biology, neurotechnology, immersive technologies, and quantum technologies among important emerging areas characterized by rapid development and uncertain future impacts (OECD, 2025).

3.1 Artificial Intelligence and Machine Learning

Artificial intelligence (AI) and machine learning are becoming important tools across scientific research. Researchers use these methods to identify patterns in large datasets, develop predictive models, classify complex information, and support experimental design. AI is being applied in fields such as drug discovery, genomics, materials science, astronomy, climate research, and biomedical science. Its ability to process large volumes of information has created opportunities for faster analysis and the development of new research questions.

AI is also changing the way researchers interact with scientific information. Machine learning systems can assist with literature analysis, image recognition, data interpretation, simulation, and hypothesis generation. However, AI-based research also requires careful evaluation because computational predictions may contain errors or reflect biases present in training data. Messeri and Crockett (2024) have warned that excessive confidence in AI-generated results may create an illusion of scientific understanding without sufficient empirical validation.

3.2 Big Data and Data-Intensive Science

The expansion of digital instruments, sensors, satellites, genomic technologies, and online scientific databases has produced unprecedented volumes of research data. This has encouraged the development of data-intensive approaches in which scientific discovery depends heavily on data collection, storage, processing, visualization, and interpretation.

High-performance computing, cloud computing, and advanced statistical methods allow researchers to analyse datasets that would be difficult to handle using conventional approaches. Data-intensive research is particularly important in genomics, climate science, astronomy, epidemiology, environmental monitoring, and social science. Open research infrastructures and FAIR principles, which emphasize data that are findable, accessible, interoperable, and reusable, are also becoming important components of modern research practice (UNESCO, 2021).

3.3 Biotechnology, Genomics, and Synthetic Biology

Biotechnology is undergoing rapid development through advances in genome sequencing, gene editing, computational biology, and synthetic biology. Researchers can now investigate biological systems at increasingly detailed molecular levels and use this information for applications in healthcare, agriculture, food production, and environmental management.

Synthetic biology combines biological knowledge with engineering principles to design or modify biological systems. Potential applications include development of new medicines, engineered microorganisms, improved agricultural systems, and biological approaches to environmental problems. At the same time, these developments require careful consideration of biosafety, biosecurity, ethical responsibility, and equitable access (OECD, 2025).

3.4 Nanotechnology and Advanced Materials

Research in nanotechnology and advanced materials is another important emerging area. Scientists are developing materials with controlled structural, electrical, optical, magnetic, and mechanical properties. Nanomaterials, two-dimensional materials, smart materials, and advanced composites are being investigated for applications in energy storage, electronics, healthcare, sensors, aerospace, and environmental technologies.

The importance of materials research is also increasing because advanced materials can support cleaner energy systems, lightweight structures, efficient electronic devices, and improved resource utilization. Increasingly, materials science is being connected with computational methods and AI to predict material properties and accelerate materials discovery. This reflects a broader movement toward technological convergence in which multiple fields contribute to the development of new research and technological solutions (OECD, 2025).

3.5 Robotics, Automation, and Intelligent Research Systems

Automation is changing both laboratory research and industrial experimentation. Robotic systems can perform repetitive experimental procedures, handle samples, collect measurements,

and support high-throughput testing. Automated systems can improve consistency and reduce the time required for repetitive tasks.

In manufacturing research, robotics is increasingly combined with sensors, AI, computer vision, and digital control systems. Similar developments are occurring in scientific laboratories, where automated platforms can support large numbers of experiments and rapidly generate experimental data. The integration of robotics with AI and other technologies is contributing to the convergence of physical and digital research systems (OECD, 2025).

3.6 Quantum Science and Technology

Quantum science and technology is emerging as an important research frontier. Quantum computing, quantum sensing, and quantum communication use properties of quantum systems to develop new approaches to information processing, measurement, and communication. Potential applications include healthcare, energy systems, scientific simulation, secure communication, and financial technologies.

Quantum technologies are still developing, and many practical applications require further research and infrastructure. Their development also raises concerns about unequal access to advanced technology and potential effects on current information security systems. UNESCO has identified quantum science and technology as an emerging field with potential relevance to healthcare, energy, agriculture, communication, and sustainable development (UNESCO, 2025).

3.7 Green and Sustainable Technologies

Sustainability has become an increasingly important direction in science and technology research. Researchers are developing renewable energy systems, energy-efficient technologies, sustainable materials, waste-reduction methods, carbon management approaches, and circular production systems. Scientific research is also being used to monitor ecosystems, model climate processes, improve resource management, and assess environmental risks.

This trend reflects the need to address interconnected environmental and socioeconomic challenges through scientific and technological solutions. Open and collaborative research can contribute to this process by allowing researchers from different regions and disciplines to share data, methods, and knowledge (UNESCO, 2021).

3.8 Open Science and Collaborative Research

Open science represents another major change in research practice. It promotes wider access to scientific publications, research data, software, methods, and other research outputs. UNESCO's Recommendation on Open Science emphasizes accessibility, transparency, collaboration, inclusion, and equitable participation in scientific research (UNESCO, 2021).

The increasing use of open repositories, shared datasets, collaborative platforms, and digital research infrastructure allows researchers to work across institutional and geographical boundaries. This approach can reduce duplication, improve reproducibility, and increase the

social value of publicly funded research. However, effective open science also requires attention to data protection, intellectual property, research quality, and unequal access to digital infrastructure.

4. Emerging Research Methodologies

The rapid development of digital technologies has changed the methods used to conduct scientific and technological research. Modern research increasingly combines experimental work with computational analysis, automation, large datasets, and digital research infrastructure. These approaches allow researchers to study complex systems, analyse large volumes of information, and improve the speed and reproducibility of scientific investigations (National Academies of Sciences, Engineering, and Medicine [NASEM], 2019).

4.1 Computational Modelling and Simulation

Computational modelling and simulation have become important alternatives and complements to conventional experimentation. Mathematical models and computer simulations can be used to examine complex biological, environmental, physical, and engineering systems. Researchers can test different conditions virtually before conducting physical experiments, reducing time and resource requirements. The integration of computational and experimental methods also supports prediction and hypothesis testing (OECD, 2015).

4.2 High-Throughput and Automated Experimentation

Automation is increasingly being introduced into laboratories and research facilities. Robotic systems can perform repetitive procedures, handle samples, collect measurements, and conduct large numbers of experiments with limited manual intervention. High-throughput approaches are particularly useful in areas such as drug discovery, genomics, materials research, and chemical sciences. They allow researchers to examine many experimental conditions within a shorter period and generate large datasets for subsequent analysis (National Research Council, 2011).

4.3 Digital Twins and Real-Time Research

Digital twin approaches create digital representations of physical objects, processes, or systems. Data obtained from sensors and monitoring devices can be used to update these digital representations and support analysis, prediction, and decision-making. Such approaches are increasingly relevant to manufacturing, engineering, healthcare, energy systems, and environmental monitoring (Jones *et al.,* 2020).

4.4 Reproducible and Transparent Research

Reproducibility has become an important methodological principle in contemporary research. Researchers are increasingly encouraged to provide detailed methods, appropriate datasets, computational procedures, and other materials required to verify or reproduce scientific findings. Transparent research practices can improve confidence in scientific results and facilitate collaboration between research groups (NASEM, 2019). Open science further supports this

transition by encouraging the sharing of publications, data, software, and research methodologies (UNESCO, 2021).

Overall, emerging methodologies are creating a more integrated research process in which experimentation, computation, automation, and data analysis work together. Their effective use requires appropriate infrastructure, researcher training, methodological transparency, and attention to scientific and ethical standards.

5. Impact on Science, Technology & Society

Emerging research paradigms are changing not only how scientific knowledge is produced but also how technological innovation reaches society. The increasing use of artificial intelligence, advanced computing, automation, biotechnology, data-intensive methods, and open research is reducing the separation between scientific discovery and technological application. These changes are creating new opportunities for faster research, improved decision-making, economic development, and solutions to environmental and social problems (OECD, 2025).

5.1 Scientific Discovery

Artificial intelligence, machine learning, large datasets, and computational modelling are improving the ability of researchers to identify patterns and generate predictions from complex datasets. AI is now being used across many scientific disciplines, including biology, medicine, materials science, chemistry, and environmental research. A large-scale analysis found that the use and potential benefits of AI in scientific research have increased substantially, particularly since 2015 (Gao & Wang, 2024). In life sciences, AI-based research has also expanded rapidly, although its development remains geographically concentrated in a limited number of countries (Schmallenbach *et al.,* 2024). These developments can increase research productivity, but they also require researchers to critically evaluate AI-generated results rather than treating computational outputs as automatically reliable.

5.2 Technological Innovation

Emerging research methods are shortening the pathway from scientific knowledge to technological development. Automated experimentation, advanced materials, biotechnology, digital systems, and computational simulation allow researchers and industries to test more possibilities and improve products more efficiently. The convergence of different technologies is also creating new innovation opportunities by combining areas such as AI, biotechnology, advanced materials, and digital technologies (OECD, 2025). This can support the development of new medicines, manufacturing processes, energy systems, communication technologies, and intelligent machines.

5.3 Healthcare and Life Sciences

Healthcare is one of the major areas affected by emerging research paradigms. AI and data-driven methods are being applied to medical diagnosis, clinical decision support, drug

development, disease surveillance, and health-system management. The World Health Organization recognizes substantial potential for AI to improve health services and research, while also stressing the need for safety, transparency, human oversight, privacy, and equitable access (World Health Organization [WHO], 2021). Biotechnology and genomic research are similarly contributing to improved disease understanding, precision medicine, and development of new therapeutic approaches.

5.4 Industry and Economy

Advanced research technologies are influencing industrial productivity, innovation, and employment. Automation and intelligent systems can improve production efficiency, quality control, resource management, and predictive maintenance. At the same time, changes in technological capabilities may alter job requirements and increase demand for digital and analytical skills. The distribution of benefits is therefore influenced by access to infrastructure, education, investment, and technological capabilities (OECD, 2025).

5.5 Environment and Sustainability

Emerging technologies also have an important role in addressing environmental challenges. Advances in renewable energy, energy storage, smart grids, low-carbon manufacturing, and computational environmental monitoring can support climate mitigation and resource efficiency. Clean-energy innovation is particularly important because several difficult-to-decarbonize sectors require new technologies and improved existing technologies to meet long-term climate objectives (International Energy Agency [IEA], 2024). Open science can further strengthen international cooperation by making research outputs, data, software, and methods more accessible and reusable (UNESCO, 2021).

6. Challenges & Ethical Considerations

The rapid development of emerging research paradigms has created important scientific and technological opportunities, but it has also introduced challenges related to research quality, ethics, security, accessibility, and responsible innovation. The increasing dependence on artificial intelligence, large datasets, automated systems, biotechnology, and advanced computing requires researchers to consider not only what can be achieved but also how research should be conducted and applied.

6.1 Research Integrity and Reproducibility

Complex computational methods and automated research systems can make scientific processes difficult to reproduce. AI-generated results may also contain errors, unsupported conclusions, or hidden biases. Researchers therefore need to maintain transparent methods, appropriate validation, documentation, and independent verification. Reproducibility is particularly important when computational models or large datasets influence scientific conclusions (National Academies of Sciences, Engineering, and Medicine [NASEM], 2019).

6.2 Data Privacy and Security

Data-intensive research often involves large volumes of personal, biological, health, and behavioural information. Improper collection, storage, sharing, or processing of such data can create privacy and security risks. Strong data governance, informed consent, access controls, and responsible data-sharing practices are therefore essential, particularly in biomedical and AI-based research (World Health Organization [WHO], 2021).

6.3 Bias and Reliability in Artificial Intelligence

AI systems can reproduce biases present in their training data or research processes. In scientific applications, excessive reliance on AI-generated outputs may also create misleading confidence in results. Researchers must therefore assess data quality, model performance, uncertainty, and limitations rather than accepting computational predictions without critical evaluation (Messeri & Crockett, 2024).

6.4 Ethical Issues in Biotechnology

Advances in genomics, synthetic biology, and gene-editing technologies raise questions concerning safety, human health, environmental effects, consent, and possible misuse. Responsible governance is required to ensure that scientific progress does not create unacceptable biological or social risks.

6.5 Equity, Intellectual Property, and Environmental Cost

Access to advanced research infrastructure is uneven across countries and institutions. High-performance computing, specialised laboratories, datasets, and skilled personnel can be expensive. Intellectual-property restrictions may further limit knowledge sharing. In addition, energy-intensive computing and large-scale technological infrastructure can contribute to environmental pressures. Open science, responsible innovation, capacity building, and sustainable research practices are therefore important for ensuring that emerging technologies provide broad social benefits (UNESCO, 2021).

7. Future Directions

The future of science and technology research will be shaped by greater integration of digital technologies, interdisciplinary approaches, automation, and open collaboration. Artificial intelligence and machine learning are expected to become more closely integrated with scientific workflows, supporting data analysis, prediction, experiment design, and knowledge discovery. However, human expertise and independent validation will remain essential for maintaining scientific reliability (Messeri & Crockett, 2024).

Future research is also likely to focus on the convergence of AI with biotechnology, advanced materials, robotics, quantum technologies, and other emerging fields. Such convergence can support new approaches to healthcare, energy, manufacturing, environmental management, and climate-related research (OECD, 2025). Automated laboratories and high-throughput

experimentation may further increase research speed by allowing large numbers of experiments to be performed and analysed with limited manual intervention.

Open and collaborative research will remain important for improving transparency, reproducibility, and international cooperation. Greater sharing of publications, datasets, software, and research infrastructure can reduce duplication and improve access to scientific knowledge (UNESCO, 2021). At the same time, future research systems will need stronger attention to data protection, cybersecurity, intellectual property, responsible AI, and ethical biotechnology.

Sustainable research should also become a priority. Energy-efficient computing, environmentally responsible laboratories, and low-carbon technologies will be increasingly important as research infrastructure expands. Finally, investment in research skills, digital literacy, interdisciplinary training, and equitable access to advanced infrastructure will be necessary to ensure that emerging scientific capabilities benefit both developed and developing regions.

Conclusion

Emerging paradigms in science and technology research are changing the way knowledge is generated, tested, shared, and applied. Artificial intelligence, machine learning, big data, biotechnology, nanotechnology, robotics, quantum technologies, and sustainable technologies are providing new tools for addressing complex scientific and societal problems. At the same time, computational modelling, automated experimentation, digital twins, and open science are improving research efficiency, collaboration, and reproducibility. These developments are strengthening connections between different scientific disciplines and between research institutions, industry, and society. However, technological progress also creates challenges related to research integrity, data privacy, algorithmic bias, intellectual property, unequal access, and environmental impacts. Therefore, future research should focus on responsible and transparent use of emerging technologies, supported by appropriate ethical frameworks and effective governance. A balanced approach that combines scientific innovation with human judgement, collaboration, sustainability, and social responsibility will be essential for ensuring that emerging research paradigms contribute to reliable knowledge, technological progress, and wider societal benefit.

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ARTIFICIAL INTELLIGENCE AND DIGITAL TWINS FOR PREDICTIVE MAINTENANCE OF AEROSPACE SYSTEMS

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Abstract

Aerospace systems operate under demanding mechanical, thermal and environmental conditions, making maintenance essential for safety, reliability and operational availability. Conventional maintenance programmes provide established inspection and servicing arrangements, but they may offer limited visibility into the evolving condition of individual components between scheduled interventions. Artificial Intelligence (AI) and digital twins offer complementary capabilities for interpreting condition-monitoring data, assessing degradation and supporting maintenance planning. AI identifies patterns within sensor measurements and maintenance records, while digital twins maintain evolving computational representations of physical assets using engineering models and operational observations. Their integration can connect anomaly detection, fault diagnosis, remaining useful life estimation and maintenance decision support within a common framework. This chapter examines maintenance strategies, relevant AI methods, digital twin updating, representative aerospace applications and implementation requirements. It presents a conceptual architecture, an asset-updating cycle and a human-guided decision process, supported by comparative tables and illustrative graphs. The graphs demonstrate degradation progression, uncertainty in remaining useful life and sensitivity to operating load without claiming experimental validation. Particular attention is given to data quality, operating-condition variability, model evaluation, cybersecurity and human oversight. The chapter concludes that dependable predictive maintenance requires traceable data, validated models, explicit uncertainty and accountable engineering decisions. AI and digital twins should support maintenance personnel within applicable approved maintenance.

Keywords: Artificial Intelligence, Digital Twins, Predictive Maintenance, Aerospace Systems, Remaining Useful Life, Condition Monitoring, Aircraft Reliability, Physics-Informed Learning.

1. Introduction

Aerospace maintenance connects engineering knowledge with the practical responsibility of keeping aircraft systems serviceable. Engines, structures, actuators and electrical equipment

experience changing loads and operating environments throughout their service lives. Their condition depends on accumulated usage, material characteristics, individual operating history and previous maintenance interventions. Components with similar operating hours may therefore exhibit different degradation patterns.

Maintenance organisations must interpret this variability while managing inspection requirements, replacement-component availability and operational schedules.

Condition-based maintenance provides an established foundation for interpreting equipment condition. Jardine *et al.* (2006) reviewed machinery diagnostics, prognostics and maintenance decision-making, emphasising the connection between condition information and intervention.

Glaessgen and Stargel (2012) presented an aerospace digital twin concept integrating simulation, vehicle health monitoring, maintenance history and fleet information. Combining these capabilities creates an opportunity to connect measured behaviour with engineering models. AI may identify a persistent departure from expected behaviour, while the twin can help investigate whether that departure is consistent with a plausible degradation mechanism.

This chapter presents a narrative review and a proposed implementation framework. It does not report new experiments. Its conceptual diagrams and illustrative graphs explain how condition monitoring, prediction, uncertainty and maintenance decisions can be connected.

2. Maintenance Strategies and Degradation Assessment

2.1 Evolution of Maintenance Strategies

Corrective maintenance responds to an identified fault or failure. Preventive maintenance follows established time or usage intervals. Condition-based maintenance uses observed equipment condition, while predictive maintenance adds a forecast of how that condition may develop.

Table 1: Comparison of Aerospace Maintenance Strategies

Maintenance Strategy	Intervention Trigger	Main Contribution	Principal Limitation
Corrective	Identified fault or failure	Restores serviceability	Action follows the occurrence of a problem
Preventive	Time, cycles or established schedule	Supports planned inspection and servicing	Individual degradation may differ from assumed patterns
Condition-based	Evidence of current equipment condition	Connects intervention with observed behaviour	Requires reliable measurements and interpretation
Predictive	Forecast of future condition	Supports advance inspection and resource planning	Requires validated forecasts and uncertainty assessment

These approaches can coexist within an aerospace maintenance programme. Their suitability depends on the component, failure mechanism, detectability of deterioration and consequences of failure.

Predictive information should support the approved maintenance programme. A model output alone does not justify extending a component's prescribed life or changing an inspection interval.

2.2 Detection, Diagnosis and Prognosis

Three functions should remain distinct. Detection identifies unusual behaviour. Diagnosis investigates its cause. Prognosis estimates its future development.

For example, increasing vibration may indicate an abnormal condition. Diagnosis must determine whether the change arises from deterioration, imbalance, changing load or a sensor issue. Prognosis then estimates the progression of the relevant mechanism.

An anomaly detector does not automatically provide a dependable remaining-life estimate. Similarly, a prognostic model developed for one failure mechanism may be unsuitable when another mechanism develops.

2.3 Degradation Progression

A degradation indicator expresses a measurable or estimated change in component condition. It may be constructed from vibration, temperature, performance loss or another relevant quantity. Its engineering meaning and relationship with the monitored failure mechanism must be established.

Graph 1 illustrates an accelerating degradation pattern using the assumed relationship:

$$D(t) = 10 + 90(t/200)^2$$

where D(t) is a dimensionless degradation index and t is operating time in hours. An illustrative maintenance threshold is set at 80 index units.

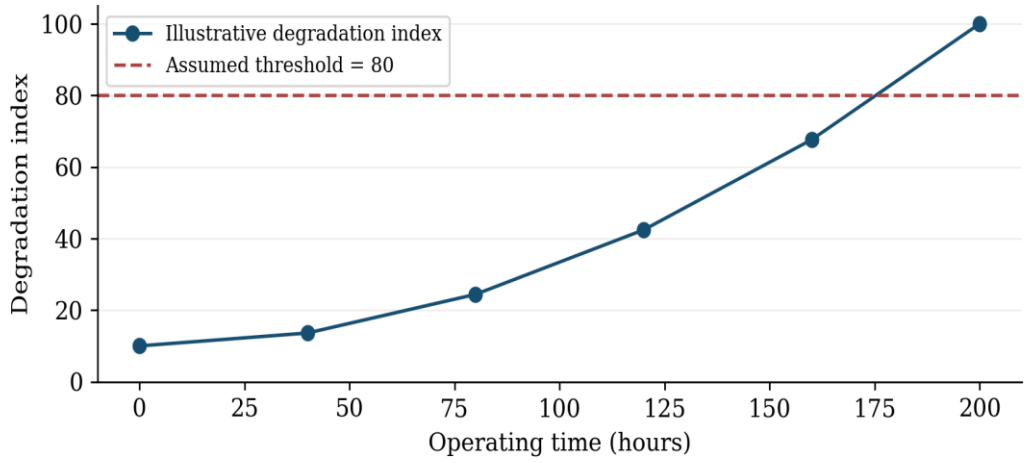


Figure 1: Illustrative component degradation trajectory and defined maintenance threshold

Under this assumed relationship, the degradation index reaches 80 at approximately 176.4 operating hours. This calculation demonstrates how a forecast can identify an approaching intervention point. Neither the equation nor the threshold represents a validated aerospace component model or an approved maintenance limit.

2.4 Remaining Useful Life

Remaining Useful Life (RUL) is the predicted interval before a component reaches a specified end-of-use criterion under stated assumptions:

$$RUL(t) = T_{limit} - t$$

The endpoint must be clearly defined. A performance threshold, a damage limit and a prescribed component life are different concepts. A useful RUL statement identifies the endpoint, units, assumed future operation and uncertainty.

Lei *et al.* (2018) reviewed machinery prognostics across the workflow from data acquisition to RUL prediction. Their review supports considering data preparation, health assessment and prediction as connected stages rather than evaluating the forecasting algorithm in isolation.

For the framework proposed here, an RUL estimate should therefore be accompanied by enough information to assess how it was obtained and whether its assumptions match the planned operation.

3. Artificial Intelligence for Condition Monitoring

3.1 Data Quality and Operating Context

AI models require measurements with reliable timestamps, units, sensor identities and component identities. Missing observations, calibration changes and maintenance events should remain visible during processing.

Operating context is equally important. Measurements recorded under different loads or flight phases may differ even when component condition remains unchanged. Data preparation should establish comparable conditions before interpreting a trend as degradation.

Engineering features can include vibration characteristics, temperature trends, pressure relationships and departures from a healthy baseline. Feature selection should consider physical relevance as well as statistical association.

3.2 Relevant AI Methods

Different methods address different maintenance questions. Supervised learning uses labelled examples, while unsupervised approaches can identify departures from familiar behaviour. Sequence models examine changes over time.

Zhao *et al.* (2019) reviewed deep learning applications in machine health monitoring, including autoencoders, convolutional networks and recurrent networks. Their review provides a foundation for selecting methods according to the available measurements and intended task.

Table 2: AI Methods, Aerospace Applications and Validation Requirements

AI method	Candidate application	Expected output	Validation requirement
Regression or tree-based model	Engine performance trending	Estimated condition or RUL	Evaluation on unseen assets
Support vector machine	Known fault patterns	Condition class	Missed faults and false classifications
Autoencoder	Unusual sensor behaviour	Anomaly score	Representative healthy-condition data
Convolutional neural network	Vibration or inspection images	Features or defect class	Independent conditions and inspections
Sequence model	Time-dependent degradation	Condition trajectory or RUL	Asset-level and chronological evaluation
Hybrid physics–data model	Engine or structural updating	Physical state and forecast	Physical consistency and uncertainty

A transparent baseline should precede a complex model. Additional complexity is justified when it improves independent performance or provides a useful engineering capability.

3.3 Generalisation and Data Leakage

Repeated observations from the same engine or component are related. Randomly dividing individual observations can place information from one asset in both training and test sets, creating an overly favourable evaluation.

The evaluation approach proposed here separates data by asset identity. It also examines changed operating conditions and preserves chronological order where future deployment is the intended use.

Scaling, feature selection and model tuning should use training data. Held-out test information should remain unavailable until final evaluation. Results should identify the asset population and operating range over which performance has been assessed.

4. Digital Twins and AI Integration

4.1 Asset-Specific Computational Representation

For this chapter, a maintenance digital twin is an asset-specific computational representation updated through operational observations and documented interventions. It can include physical models, estimated condition, uncertainty and maintenance history.

Li *et al.* (2022) reviewed digital twins in aerospace and discussed the importance of distinguishing a twin from a digital model or digital shadow. Their discussion highlights data acquisition and interaction with the represented asset as important elements of implementation.

The required model detail depends on the decision. A component-level model may be sufficient for a bearing investigation, whereas structural assessment may require information about geometry, loading and material response. The objective is a computational representation suitable for the maintenance question, with a documented relationship to its physical asset.

4.2 State Updating and Maintenance Feedback

The full condition of a component is rarely directly observable. A twin must estimate hidden quantities using incomplete measurements.

Kapteyn *et al.* (2021) presented a probabilistic formulation for interacting asset–twin systems and demonstrated a structural twin for an unmanned aerial vehicle. Their work illustrates how observations, evolving states and decisions can be represented consistently.

A simplified state-estimation structure is:

$$x_{t+1} = f(x_t, u_t, \theta) + w_t$$

$$y_t = h(x_t, u_t, \theta) + v_t$$

Here, Xt represents asset state, ut operating conditions, θ model parameters and Yt measurements. The terms Wt and Vt represent modelling and measurement uncertainty.

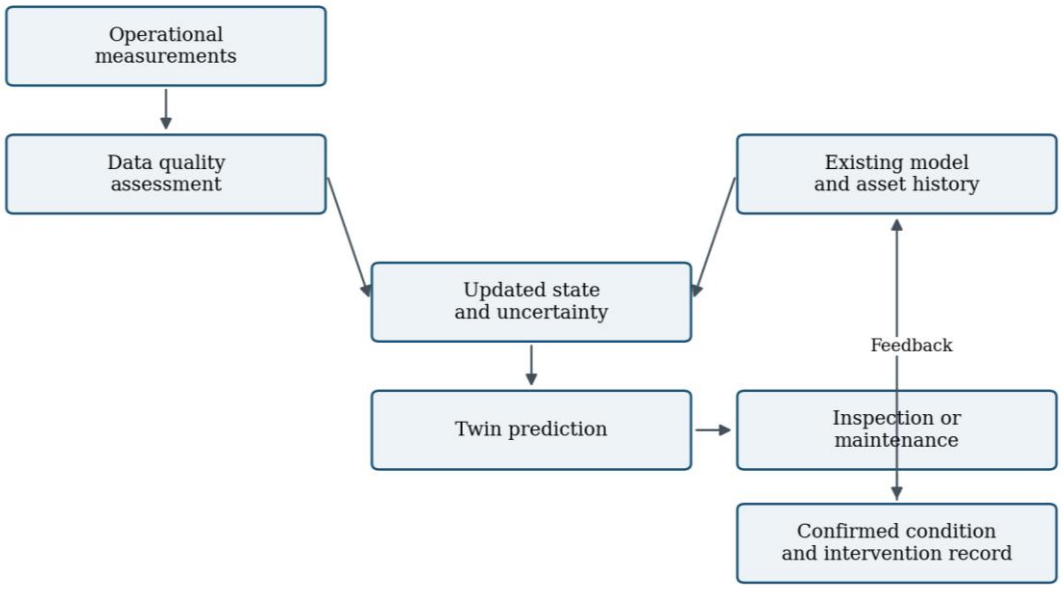


Figure 2: Digital twin updating cycle incorporating operational data and maintenance feedback

After repair or replacement, the twin should represent the resulting condition. It should not continue forecasting from an obsolete pre-maintenance state.

4.3 Physics-Informed and Hybrid Learning

Physical models and data-driven models have complementary limitations. A physical model may omit relevant behaviour, while a data-driven model may lack representative examples.

Raissi *et al.* (2019) introduced physics-informed neural networks that incorporate governing differential equations into neural-network learning. This provides a methodological foundation for combining observations with physical relationships.

Karniadakis *et al.* (2021) examined the broader field of physics-informed machine learning, including the integration of mathematical models and observations, alongside continuing challenges.

Candidate maintenance applications include estimating degradation parameters, learning corrections to an engineering model and constraining predictions to meaningful ranges. The framework proposed here requires checking both the suitability of the physical assumptions and the independent performance of the resulting model.

4.4 Integrated Architecture

The proposed architecture separates data preparation, computational analysis, evidence assessment and engineering action.

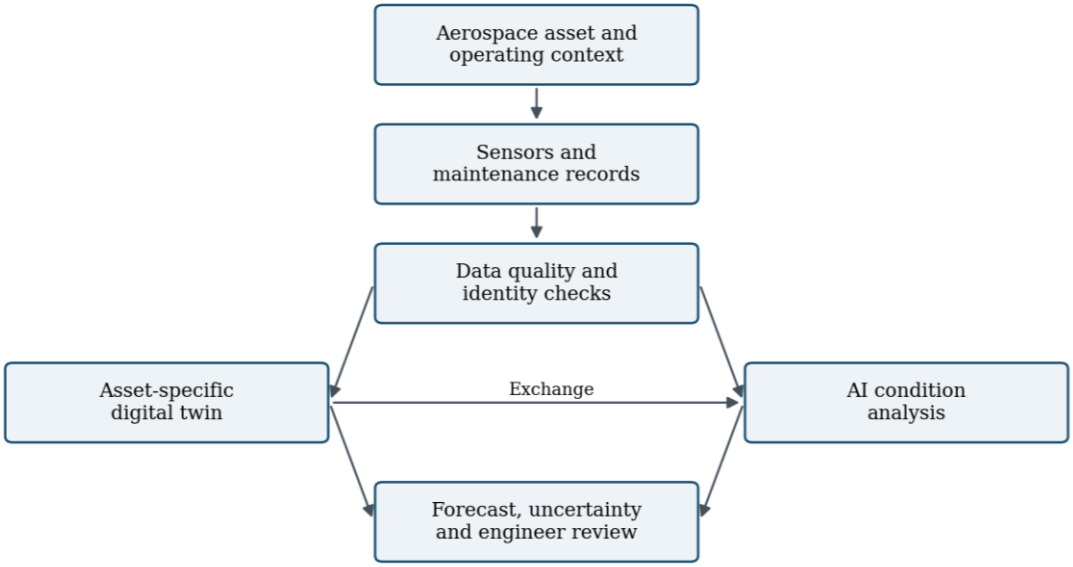


Figure 3: Integrated AI–digital twin architecture for aerospace predictive maintenance

The AI component analyses patterns, while the twin maintains the asset representation. Their combined outputs should include uncertainty and supporting evidence. Confirmed inspection results provide feedback for subsequent analysis.

5. Aerospace Applications and Evidence

5.1 Aircraft Engines

Engine monitoring can examine interacting thermal, pressure, speed and vibration measurements. A candidate twin compares measured behaviour with expected behaviour under comparable operating conditions. AI can assist with detecting persistent changes across multiple channels.

Saxena and Goebel (2008) provided the Turbofan Engine Degradation Simulation Data Set through the NASA Prognostics Data Repository. These C-MAPSS datasets contain simulated degradation trajectories under combinations of operating conditions and fault modes.

Saxena *et al.* (2008) described the associated damage propagation modelling approach for engine run-to-failure simulation. The dataset and methodological publication provide a foundation for reproducible prognostics research. Their simulated trajectories should not be presented as observed operational engine failures.

Arias Chao *et al.* (2021) presented a further synthetic engine dataset incorporating realistic flight conditions. It enables research under varied operational histories, while requiring separate validation before findings are transferred to operational fleets.

5.2 Structures and Composite Components

A proposed structural application connects strain, vibration and inspection observations with a model of structural response. The research question is whether measured changes are consistent with altered stiffness or damage.

Controlled specimens and ground-test components provide opportunities for independent verification. Evaluation should examine damage-location uncertainty, environmental sensitivity and agreement with inspection findings.

5.3 Actuators and Rotating Components

Actuator and rotating-component demonstrators allow controlled changes in operating conditions. Depending on the equipment, measurements can include current, position, pressure, temperature and vibration.

A candidate twin represents expected behaviour under a known command or load. AI can investigate persistent differences between expected and measured responses. Laboratory results should remain identified as laboratory evidence.

5.4 Batteries and Electrical Systems

A proposed battery twin combines electrical and thermal measurements with a degradation model. Condition assessment should distinguish available energy, power capability and component health because they support different decisions.

NASA's prognostics repository includes battery, bearing and composite datasets as research resources. Each dataset must be interpreted according to its experimental or simulation conditions. Saxena and Goebel (2008) provide the corresponding engine degradation dataset discussed in Section 5.1.

5.5 Industrial Practice

Rolls-Royce (n.d.) describes its IntelligentEngine platform as connecting engine health and performance information with digital capabilities for maintenance-demand prediction. This

provides an industrial example of integrating asset information with maintenance services. Its description does not establish a universal percentage improvement in cost or reliability.

6. Illustrative Prediction and Maintenance Planning

6.1 Remaining Useful Life and Uncertainty

A point estimate can conceal substantial uncertainty. Graph 2 illustrates an assumed RUL forecast at four observation times. For illustration:

$$\widehat{RUL}(t) = 180 - t$$

$$RUL_{\text{lower}}(t) = 140 - t$$

$$RUL_{\text{upper}}(t) = 225 - t$$

These relationships are constructed examples. The bounds represent a hypothetical 90% predictive interval; no empirical coverage has been established.

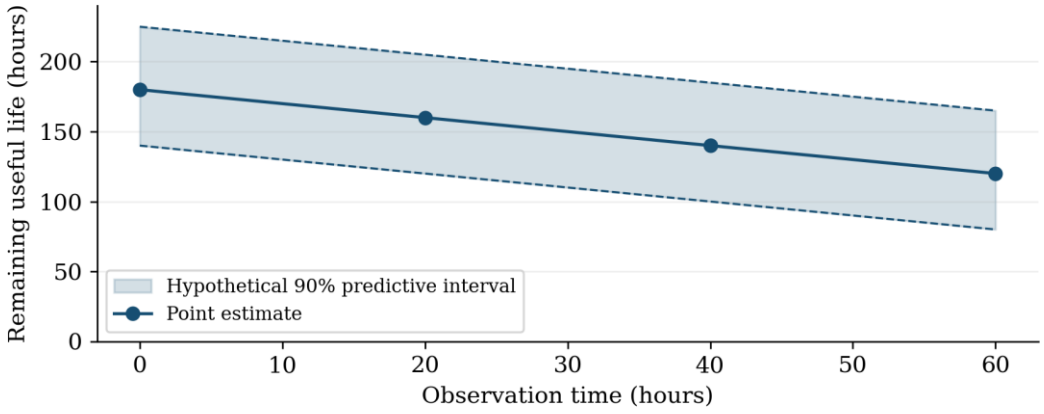


Figure 4: Illustrative remaining useful life forecast with a predictive uncertainty band

At the final observation, the point estimate is 120 hours and the assumed interval is 80–165 hours. The shaded region represents the illustrative interval.

If the next planned maintenance opportunity follows 70 additional operating hours, the difference between the lower bound and planned workload is:

$$80 - 70 = 10 \text{ hours}$$

This difference is not an established safety margin. It identifies the need to review uncertainty, future loading, sensor credibility and applicable maintenance instructions.

6.2 Effect of Operating Load

Future operation influences a degradation forecast. Graph 3 demonstrates this sensitivity through an assumed inverse relationship:

$$RUL(L) = \frac{120}{L}$$

where L is a dimensionless load factor relative to an assumed baseline.

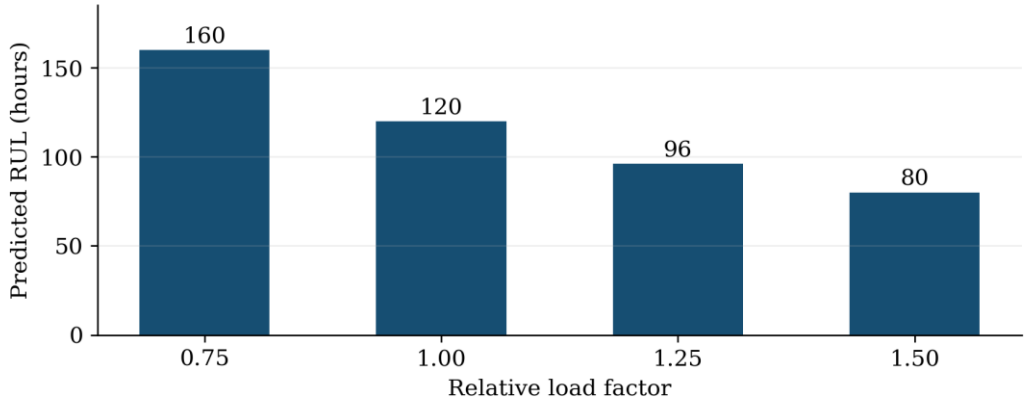


Figure 5: Illustrative effect of operating load on predicted remaining useful life

The example produces RUL values of 160, 120, 96 and 80 hours. It demonstrates why a forecast must state its assumed operating conditions. Actual load–degradation relationships may differ substantially.

6.3 Human-Guided Decision Process

An alert should initiate a structured review. Engineers should examine data quality, supporting measurements, operating context and consistency with inspection evidence.

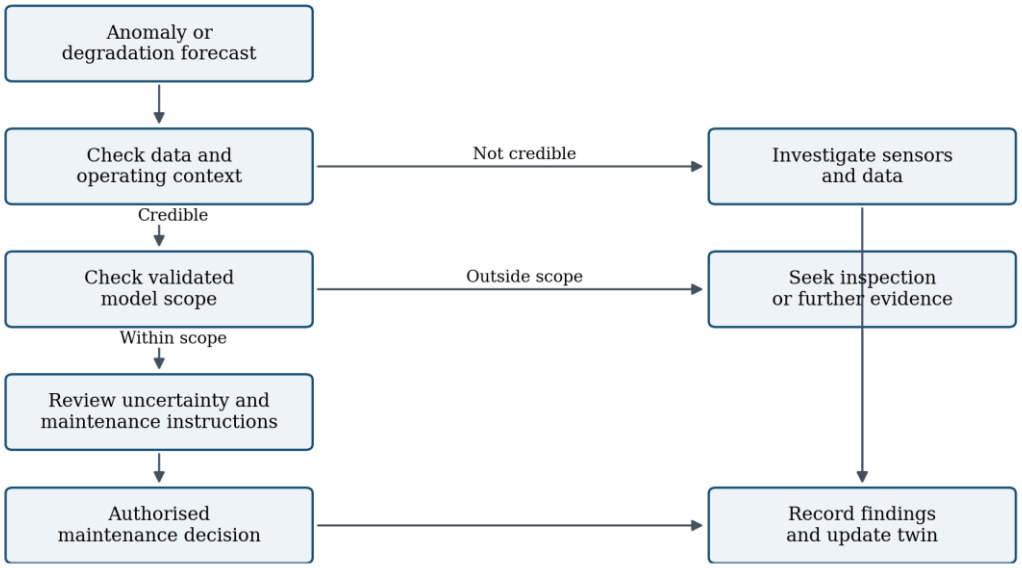


Figure 6: Human-guided maintenance decision process from anomaly detection to intervention

Possible outcomes include additional monitoring, inspection, maintenance or rejection of an unsupported prediction. The appropriate action depends on the component and the applicable approved processes.

7. Validation and Implementation

7.1 Prediction Accuracy and Decision Usefulness

Validation should examine prediction accuracy, uncertainty quality and practical usefulness.

For RUL prediction:

$$MAE = \frac{1}{N}\sum_{i=1}^{N}\left|\widehat{RUL}_i - RUL_i\right|$$

Mean Absolute Error provides an average discrepancy but does not distinguish potentially consequential overestimation from underestimation. Evaluation should also report error direction and performance near decision thresholds.

Saxena *et al.* (2009) examined prognostic performance metrics that account for prediction timing and uncertainty, including prognostic horizon and alpha–lambda performance. These complement average errors by assessing when forecasts become useful and whether they remain within defined accuracy bounds.

The evaluation framework proposed here also reports false alarms, missed detections, interval coverage and interval width. It assesses whether predictive information arrives early enough to support inspection, procurement or maintenance planning.

7.2 Human Oversight and Accountability

The maintenance interface should identify supporting measurements, assumptions, uncertainty and model version. Personnel should be able to document acceptance, rejection and inspection outcomes. European Union Aviation Safety Agency (2023) provides a human-centred direction for AI in aviation through its Artificial Intelligence Roadmap 2.0. The roadmap addresses safety and ethical considerations but does not constitute approval of a particular maintenance application. Tabassi (2023) presents the NIST AI Risk Management Framework as voluntary guidance for managing AI risks. It can inform development governance, while aviation-specific requirements require separate assessment. Within the proposed framework, models generate evidence and authorised personnel determine maintenance action.

7.3 Data Integrity and Cybersecurity

Incorrect component identities, altered maintenance records or unauthorised model changes can undermine predictions. The proposed implementation includes controlled access, traceable model versions and documented data transfers. Unavailable sensors or connectivity should trigger a defined degraded mode. Personnel should understand which information remains dependable and which existing procedures apply when predictive support is unavailable.

7.4 Staged Implementation Pathway

Implementation should begin with a specific maintenance problem and a clear decision boundary.

Progression should depend on evidence. Completion of a software prototype alone does not establish readiness for maintenance use.

Table 3: Staged Implementation of AI–Digital Twin Maintenance Systems

Stage	Main Activity	Evidence Required
Define the use case	Identify component, mechanism and intended decision	Clear scope and decision boundary
Establish a baseline	Assess existing indicators and simple models	Reproducible baseline performance
Audit the data	Check identity, quality, context and interventions	Documented fitness for the task
Introduce controlled support	Use reviewed outputs within procedures	Accepted validation and responsibility arrangements
Monitor and update	Track drift, errors and feedback	Continuing suitability for intended use

Source: Proposed implementation framework developed for this chapter.

8. Research Challenges and Future Directions

8.1 Transfer Across Assets

Models may encounter different sensors, materials, workloads and maintenance practices when transferred to new assets. Future studies should examine these changes explicitly and report their effects on prediction quality. A useful research design evaluates previously unseen assets and operating conditions, identifying where recalibration or further evidence is required.

8.2 Incomplete Degradation Histories

Operational components may be repaired or removed before failure. Their records should not automatically be treated as complete run-to-failure trajectories.

Future research should distinguish replacement, repair and continuing service. It should also examine how maintenance interventions change the state represented by the twin.

8.3 Maintenance and Resource Planning

Accurate forecasts may offer limited value when inspection capacity or replacement components are unavailable. Future systems should connect condition estimates with realistic planning constraints while retaining applicable maintenance requirements. Decision usefulness should be assessed through clearly defined planning outcomes rather than prediction accuracy alone.

8.4 Efficient and Interpretable Twins

The computational detail of a twin should match its decision purpose. Research can investigate reduced models that preserve the quantities relevant to condition assessment.

Explanations should help engineers inspect physical consistency, data quality and assumptions. Their usefulness depends on whether they support an engineering check.

8.5 Academic Research Opportunities

A practical study can begin with a bearing rig, actuator demonstrator, battery arrangement or composite specimen. Comparing a simple baseline, a data-driven model and a hybrid model under the same conditions provides a useful research structure.

Research proposals should specify the data source, reference measurements, decision target and validation plan. These details distinguish a demonstrator from a validated maintenance system.

Conclusion

AI and digital twins provide complementary capabilities for aerospace predictive maintenance. AI assists with identifying patterns and estimating degradation, while digital twins connect observations with asset-specific models and maintenance histories.

The proposed framework places data quality, uncertainty assessment and human review between computational prediction and maintenance action. Inspection findings and documented interventions update the asset representation and support continuing evaluation.

The three figures explain the updating cycle, integrated architecture and decision process. The three tables organise maintenance strategies, candidate AI methods and implementation stages. The three illustrative graphs demonstrate degradation progression, prediction uncertainty and sensitivity to operating load without claiming measured performance.

Dependable deployment requires validation under the intended conditions and assessment of practical decision value. A staged implementation pathway can help researchers and maintenance organisations develop predictive support that strengthens engineering judgement and contributes to safety, reliability and operational availability.

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DATA-DRIVEN ARTIFICIAL INTELLIGENCE METHODS, APPLICATIONS AND FUTURE PERSPECTIVES

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Abstract

Data-driven artificial intelligence (AI) has emerged as a major approach for developing intelligent systems capable of learning from large and diverse datasets. The effectiveness of AI increasingly depends on the availability, quality, and appropriate use of data throughout the stages of data collection, preprocessing, model development, evaluation, and deployment. This chapter presents an overview of the foundations, methods, applications, challenges, and future perspectives of data-driven AI. It discusses major approaches including machine learning, deep learning, generative AI, data analytics, and predictive modelling, with emphasis on their role in converting complex datasets into useful predictions and decision-support systems. Applications across healthcare, agriculture, education, finance, business, smart cities, and industrial systems are examined through practical examples. The chapter also highlights major concerns related to data quality, algorithmic bias, privacy, cybersecurity, explainability, and accountability. Future directions including data-centric AI, edge intelligence, federated learning, multimodal AI, and privacy-preserving technologies are considered. Overall, effective data-driven AI requires not only advanced computational methods but also reliable data, responsible governance, human oversight, and continuous evaluation to ensure accurate, secure, fair, and socially beneficial outcomes.

Keywords: Data-Driven AI, Machine Learning, Deep Learning, Generative AI, Artificial Intelligence Applications.

1. Introduction

Artificial Intelligence (AI) has developed rapidly with the increasing availability of digital data, improved computing capacity, and advances in machine learning algorithms. Modern AI systems increasingly depend on large and diverse datasets to identify patterns, generate predictions, support decisions, and automate complex tasks. This has led to the development of data-driven artificial intelligence, in which the quality, quantity, diversity, and relevance of data play a central role in determining system performance. Unlike traditional approaches that depend heavily on manually defined rules, data-driven AI allows computational models to learn relationships and patterns directly from available data (Kumar *et al.,* 2023).

The importance of data has become particularly evident with the growth of machine learning and deep learning. Data may be obtained from sensors, Internet of Things (IoT) devices, scientific experiments, healthcare systems, business transactions, digital platforms, satellite observations, and other sources. These datasets can contain structured information as well as text, images, audio, and video. However, increasing the volume of data alone does not guarantee better AI performance. Data may contain missing values, errors, duplication, noise, outdated information, or sampling bias. Therefore, data quality assessment, cleaning, preprocessing, and appropriate representation are essential components of successful AI development (Zhu *et al.,* 2025). Recent research also identifies data-centric approaches, including data preprocessing, quality assessment, data augmentation, and improved data management, as important methods for developing reliable AI systems (Kumar *et al.,* 2023).

Data-driven AI has applications across healthcare, agriculture, education, finance, manufacturing, transportation, environmental monitoring, and smart cities. At the same time, issues related to privacy, fairness, transparency, security, and bias require careful consideration. AI risk-management frameworks therefore emphasize trustworthy, reliable, explainable, privacy-enhanced, and fair AI systems (Tabassi, 2023).

This chapter examines the major methods of data-driven AI, its applications across important sectors, key challenges, and future perspectives for developing reliable and responsible intelligent systems.

2. Foundations of Data-Driven AI

Data-driven Artificial Intelligence (AI) is based on the interaction of data, algorithms, computational models, and learning processes. Data provide the information from which AI systems identify patterns and relationships, while algorithms determine how this information is processed to produce predictions or decisions. The effectiveness of a data-driven AI system therefore depends on both the quality of available data and the suitability of the selected learning method (Jordan & Mitchell, 2015).

2.1 DATA

Data are the basic input for AI systems and may be collected from sensors, databases, websites, satellites, mobile devices, scientific experiments, healthcare records, and Internet of Things (IoT) devices. They may be structured, such as numerical records and tables, or unstructured, such as text, images, audio, and video. Large datasets can improve the ability of AI models to recognize complex patterns, although data quality, completeness, diversity, and representativeness remain important factors (Sambasivan *et al.,* 2021).

2.2 Algorithms

Algorithms provide systematic procedures for processing data and learning from it. Common approaches include linear regression, decision trees, random forests, support vector machines,

clustering methods, neural networks, and transformer-based models. The selection of an algorithm depends on the type of data, research objective, computational resources, and required level of accuracy.

2.3 Models

An AI model is a trained computational system that represents patterns learned from data. During training, model parameters are adjusted to reduce errors between predicted and observed outcomes. A well-developed model should perform effectively on new data rather than simply memorizing the training dataset. Proper validation and testing are therefore essential for assessing generalization and reliability (Goodfellow *et al.,* 2016).

2.4 Learning

Data-driven AI commonly uses supervised, unsupervised, semi-supervised, and reinforcement learning**.** Supervised learning uses labelled examples for prediction or classification, whereas unsupervised learning identifies patterns within unlabelled data. Semi-supervised learning combines labelled and unlabelled information, while reinforcement learning learns through interactions and feedback. Together, these approaches provide the foundation for developing intelligent systems capable of prediction, classification, pattern recognition, and decision support (LeCun *et al.,* 2015).

3. Major Methods and Approaches

Data-driven Artificial Intelligence (AI) uses computational methods to learn patterns from data and generate predictions, classifications, recommendations, or new content. The major approaches include machine learning (ML), deep learning (DL), generative AI, and data analytics. These methods differ in their learning mechanisms, data requirements, and practical applications, but they increasingly work together in modern intelligent systems.

3.1 Machine Learning

Machine learning is one of the fundamental approaches to data-driven AI. ML algorithms learn relationships from existing datasets and use these relationships to make predictions or decisions on new observations. Supervised learning is commonly used when labelled data are available and includes methods such as linear regression, logistic regression, decision trees, random forests, and support vector machines. Unsupervised learning works with unlabeled data and is used for clustering, dimensionality reduction, and pattern discovery. Reinforcement learning allows an agent to learn through interactions with an environment by receiving rewards or penalties (Jordan & Mitchell, 2015).

3.2 Deep Learning

Deep learning uses multi-layer artificial neural networks to learn increasingly complex representations from data. Convolutional neural networks have been widely used for image and video analysis, while recurrent neural networks have been applied to sequential and time-

dependent data. More recently, transformer architectures have become important for language, vision, and multimodal applications because they can model relationships between different elements of large datasets (LeCun *et al.,* 2015; Vaswani *et al.,* 2017). Deep learning has contributed significantly to advances in computer vision, natural language processing, speech recognition, and scientific data analysis.

3.3 Generative AI

Generative AI represents an important development in data-driven systems because it can create new content based on patterns learned from training data. Large language models can generate and process text, while other generative models can produce images, audio, video, software code, and synthetic datasets. Transformer-based architectures have played a major role in the development of modern generative AI systems (Vaswani *et al.,* 2017). Generative AI is increasingly used for content creation, education, research assistance, software development, and data augmentation. However, generated outputs may contain factual errors, bias, or inappropriate content, requiring careful evaluation before practical use.

3.4 Data Analytics and Predictive Approaches

Data analytics provides methods for converting large datasets into useful information for decision-making. Descriptive analytics examines existing patterns, predictive analytics estimates future outcomes, and prescriptive approaches support decisions by comparing possible actions. When combined with ML, analytics can identify trends and provide automated predictions in areas such as healthcare, agriculture, finance, manufacturing, and environmental monitoring.

3.5 Integration of Methods

Modern AI applications increasingly combine several approaches. For example, a smart agricultural system may use data analytics to identify crop trends, ML to predict disease risk, and deep learning to analyze crop images. The selection and combination of methods should depend on the nature of the data, the intended application, computational requirements, and the level of accuracy and reliability required.

4. Data Preparation and Model Development

The performance of a data-driven Artificial Intelligence (AI) system depends strongly on how data are collected, prepared, processed, and used during model development. Even advanced AI algorithms can produce unreliable results when the input data are incomplete, noisy, biased, or poorly represented. Therefore, data preparation is an important stage in the development of reliable AI applications (Sambasivan *et al.,* 2021).

4.1 Data Collection

Data collection involves obtaining relevant information from suitable and reliable sources. Common sources include databases, sensors, Internet of Things (IoT) devices, satellite systems, scientific experiments, electronic records, websites, and digital platforms. The collected data

should represent the target population or application as accurately as possible. Adequate data diversity is also important because models trained on narrow datasets may perform poorly when applied to new situations.

4.2 Data Preprocessing

Raw data generally require preprocessing before they can be used for model development. Important activities include removing duplicate records, correcting errors, handling missing values, reducing noise, and converting data into suitable formats. Numerical variables may require normalization or standardization, while categorical information may need appropriate encoding. For image, text, and audio data, preprocessing may include resizing, tokenization, feature extraction, or noise reduction. Careful preprocessing can improve model performance and reduce errors caused by poor-quality data (Kumar *et al.,* 2023).

4.3 Model Training

After preprocessing, datasets are commonly divided into training, validation, and testing sets. The training dataset is used to learn model parameters, while validation data help in selecting model settings and reducing overfitting. The test dataset is reserved for evaluating performance on previously unseen data. Depending on the objective, researchers may use machine learning, deep learning, or generative AI methods. Model selection should consider data characteristics, computational requirements, expected accuracy, and the intended application.

4.4 Model Evaluation

Model evaluation determines whether an AI system provides reliable results. Classification models can be assessed using accuracy, precision, recall, and F1-score, whereas regression models may use measures such as mean absolute error and root mean squared error. Evaluation should also consider robustness, fairness, and performance across different groups or conditions. Continuous monitoring after deployment is important because data patterns may change over time. A systematic data and model development process therefore supports more reliable and responsible AI systems (Tabassi, 2023).

5. Applications of Data-Driven AI

Data-driven artificial intelligence is increasingly applied across sectors where large volumes of structured and unstructured data can support prediction, classification, optimization, and decision-making. The effectiveness of these systems depends on the availability, quality, and representativeness of data, as well as appropriate model selection and evaluation. Major applications are discussed below.

5.1 Healthcare

Healthcare is one of the important application areas of data-driven AI. Machine learning models can analyze electronic health records, medical images, laboratory results, and physiological data to support disease prediction and diagnosis. Deep learning techniques, particularly convolutional

neural networks, have been widely investigated for medical image analysis, including the identification of abnormalities in radiological and pathological images. AI can also contribute to personalized treatment by combining patient characteristics, clinical history, and treatment-response data. However, differences in healthcare datasets and concerns regarding privacy, bias, and clinical validation remain important challenges (Topol, 2019; Rajpurkar *et al.,* 2022).

5.2 Agriculture

In agriculture, data-driven AI combines information from satellites, drones, sensors, weather stations, and farm records to improve crop management. Image-based models can identify crop diseases and nutrient deficiencies, while predictive models can estimate crop yield using environmental and historical production data. AI-based pest monitoring can support early detection of insect infestations and help farmers apply control measures more efficiently. Precision agriculture therefore provides an important example of how data-driven models can support resource optimization and sustainable production (Benos *et al.,* 2021). Integration of AI with Internet of Things devices can further enable near-real-time monitoring of agricultural conditions.

5.3 Education

Educational institutions generate data through learning management systems, online assessments, attendance records, and student interactions. Data-driven AI can use these data to develop personalized learning pathways, predict student performance, identify learners who may require additional support, and provide intelligent tutoring. Such systems can help teachers understand learning patterns and adapt instructional strategies. At the same time, the use of student data requires careful attention to privacy, transparency, fairness, and responsible data governance.

5.4 Finance and Business

Financial institutions use data-driven AI for fraud detection, credit assessment, risk analysis, customer segmentation, and market forecasting. Machine learning models can identify unusual transaction patterns that may indicate fraudulent activity. Businesses also use predictive analytics to forecast demand, optimize inventory, understand customer behavior, and improve supply-chain management. These applications demonstrate the value of combining historical data with continuously generated transactional information. Nevertheless, model interpretability and fairness are particularly important when AI influences financial decisions.

5.5 Smart Cities and Industry

Smart cities use data from traffic cameras, GPS systems, environmental sensors, energy meters, and public infrastructure to improve urban management. AI can support traffic prediction, route optimization, energy management, waste-management planning, and public-service delivery. In manufacturing, data-driven AI is used for predictive maintenance, quality inspection, process

optimization, and industrial automation. Sensor data can help predict equipment failure before major breakdowns occur, reducing downtime and maintenance costs. Thus, integration of AI with IoT, cloud computing, and edge computing is creating increasingly intelligent industrial and urban systems.

Table 2: Major applications of data-driven AI across sectors

Sector	Major Data Sources	Representative AI Applications
Healthcare	Medical records, images, laboratory data	Diagnosis, prediction, personalized treatment
Agriculture	Satellite, drone, sensor and weather data	Disease detection, yield prediction, pest monitoring
Education	Student records, assessments, LMS data	Personalized learning, performance prediction
Finance and business	Transaction and customer data	Fraud detection, risk assessment, forecasting
Smart cities	Traffic, energy and environmental sensors	Traffic management, energy optimization
Industry	Machine and production data	Predictive maintenance, quality control, automation

Overall, data-driven AI has moved from experimental applications toward practical decision-support systems across diverse sectors. Its future value will depend not only on increasingly powerful algorithms but also on reliable data infrastructures, responsible governance, human oversight, and continuous evaluation of model performance.

6. Challenges and Ethical Considerations

Although data-driven artificial intelligence provides significant benefits, its widespread use also creates technical, ethical, social, and governance challenges. The reliability of AI systems depends strongly on the quality of data, the design of algorithms, and the way models are deployed and monitored.

6.1 Bias and Fairness

Bias can enter AI systems through incomplete, unbalanced, or historically biased datasets. When training data do not adequately represent different populations, models may produce systematically different outcomes for particular groups. Such bias is particularly concerning in healthcare, education, employment, and financial services. Therefore, dataset diversity, fairness assessment, representative sampling, and continuous model evaluation are important for reducing discriminatory outcomes (Sambasivan *et al.,* 2021).

6.2 Privacy and Data Protection

Data-driven AI frequently requires large amounts of personal, behavioural, medical, financial, or location-related information. Improper collection, storage, or sharing of such data can create privacy risks. Data minimization, anonymization, access controls, secure storage, and privacy-preserving machine learning approaches can help reduce these risks. Organizations must also ensure that data processing follows applicable legal and institutional requirements.

6.3 Data Quality and Reliability

Poor-quality data can directly affect model performance. Missing values, duplicate records, incorrect labels, measurement errors, and inconsistent formats may produce unreliable predictions. Data quality should therefore be assessed before and during model development. Continuous monitoring is also necessary because changes in real-world data can cause data drift and reduce model accuracy (Kumar *et al.,* 2023).

6.4 Security

AI systems can be affected by cyberattacks, manipulated training data, unauthorized access, and adversarial inputs. Security risks can become more serious when AI systems are connected to critical infrastructure, healthcare networks, financial systems, or industrial equipment. Secure data pipelines, authentication, monitoring, testing, and risk management are therefore essential (Tabassi, 2023).

6.5 Explainability and Accountability

Complex AI models, particularly deep neural networks, can be difficult to interpret. Lack of explainability may reduce user confidence and make it difficult to identify errors or assign responsibility for harmful decisions. Explainable AI approaches can provide information about model predictions and support human oversight. Responsible deployment therefore requires a balance between predictive performance, transparency, fairness, security, and accountability.

7. Future Perspectives

Data-driven artificial intelligence is expected to develop rapidly as data infrastructures, computational resources, and learning algorithms continue to improve. Future progress will increasingly focus on making AI systems more efficient, reliable, adaptable, and responsible.

7.1 Data-Centric and High-Quality AI

Future AI development is likely to place greater emphasis on improving datasets rather than relying only on increasingly complex models. Automated data cleaning, better annotation, representative sampling, and continuous data-quality monitoring can improve model reliability. Data-centric approaches are therefore expected to become an important component of AI development (Kumar *et al.,* 2023).

7.2 Edge AI and Real-Time Intelligence

The integration of AI with edge computing and Internet of Things devices will enable data to be processed closer to where it is generated. This can reduce communication delays, bandwidth requirements, and dependence on centralized cloud systems. Edge AI has particular potential in smart agriculture, healthcare monitoring, autonomous systems, and industrial automation.

7.3 Federated and Privacy-Preserving Learning

Federated learning allows models to be trained across distributed datasets without requiring all raw data to be transferred to a central location. This approach may become increasingly valuable for healthcare, finance, and other applications involving sensitive information. Privacy-preserving techniques can further support secure data utilization (Kairouz *et al.,* 2021).

7.4 Multimodal and Generative AI

Future systems will increasingly combine text, images, audio, video, sensor information, and other data types. Multimodal AI can support more comprehensive analysis, while generative AI can assist in content creation, simulation, and synthetic-data generation. These developments will require stronger evaluation methods and safeguards against misinformation and misuse.

7.5 Responsible and Explainable AI

Future data-driven AI systems will need greater transparency, fairness, security, and human oversight. Explainable models and systematic risk assessment can improve trust and accountability. Overall, the future of data-driven AI will depend on combining technological innovation with high-quality data, privacy protection, responsible governance, and meaningful human involvement.

Conclusion

Data-driven artificial intelligence has become an important approach for developing intelligent systems that can learn from large and diverse datasets. The effectiveness of these systems depends on the complete process of data collection, preparation, analysis, model development, evaluation, and deployment. Machine learning, deep learning, generative AI, and predictive analytics provide powerful methods for converting data into useful information and supporting decision-making across healthcare, agriculture, education, finance, business, industry, and smart cities.

However, the expansion of data-driven AI also creates important challenges related to data quality, bias, privacy, cybersecurity, transparency, and accountability. Addressing these issues requires reliable data practices, appropriate technical safeguards, responsible governance, and meaningful human oversight. Future developments will increasingly combine high-quality data with edge computing, federated learning, multimodal systems, and privacy-preserving technologies. Overall, the future of AI will depend not only on more advanced algorithms, but

also on trustworthy data, responsible innovation, and effective integration of AI with human expertise.

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TURNING CO_2 INTO VALUABLE CHEMICALS: THE CHEMISTRY AND TECHNOLOGY OF ELECTROCHEMICAL CARBON UTILIZATION

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Abstract
This chapter introduces the basic principles of electrochemical reduction CO_2 and influence of catalyst influencing reaction pathways and product formation. It also describes commonly used electrolyzer configurations, including H-type cells, flow cells, gas-diffusion electrodes, and membrane-electrode assemblies, highlighting their advantages and roles in improving process performance. The formation of products such as carbon monoxide, formate, methanol, methane, ethylene, and ethanol is discussed together with their industrial relevance. In addition, the chapter examines key challenges, including energy consumption, catalyst stability, product separation, and scale-up, and considers the importance of life-cycle and techno-economic assessments in evaluating the practicality and sustainability of CO_2 conversion technologies.
Keywords: Electrochemical CO_2 Reduction, Electrocatalysis, Carbon Capture and Utilization.

1. Introduction

Carbon dioxide is an important greenhouse gas and is also a possible source of carbon for producing useful chemicals. Most CO_2 emissions come from activities such as burning fossil fuels and from industries such as cement, steel, chemical, and plastic production. Approximately 4×10^{10} tonnes (40 billion tonnes) of CO_2 are emitted globally each year from fossil fuel combustion and industrial activities. Atmospheric CO_2 concentrations have increased from about 370 ppm in 2000 to approximately 430 ppm in 2026 and could exceed 500 ppm later in this century under high-emission scenarios.

At present global emission levels (~4×10^{10} tonnes CO_2 per year), the amount of CO_2 released corresponds to 9.09 x 10^{40} moles of CO_2. One possible strategy to mitigate atmospheric CO_2 accumulation is to convert captured CO_2 into useful fuels and chemicals. Methane and methanol are attractive options, with methanol offering advantage being liquid fuel and an efficient hydrogen carrier. Renewable hydrogen produced from water can react with captured CO_2 to synthesize methanol, which can subsequently be used in fuel cells or combustion engines. There are several ways to convert CO_2, including thermochemical, photochemical, biochemical, photoelectrochemical, and electrochemical methods. Among these, electrochemical conversion is

particularly interesting because it can use electricity to convert CO_2 into fuels and chemical products under relatively mild conditions.

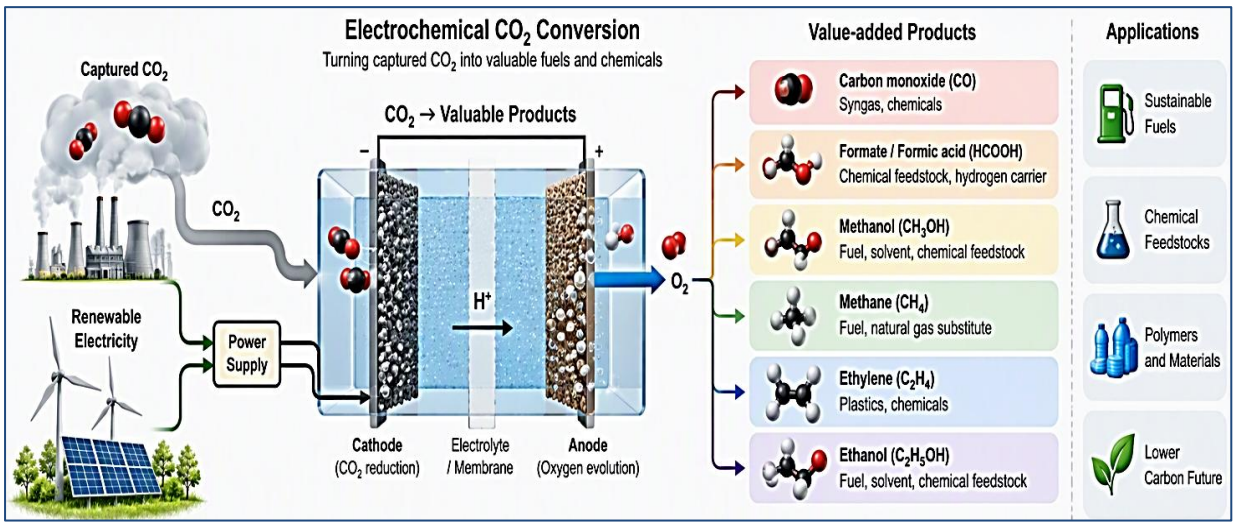


Figure 1: Electrochemical conversion of CO_2 into value-added fuels and chemicals using electricity.

Electrochemical CO_2 conversion also known as CO_2RR, is the conversion of CO_2 to more reduced chemical species using electrical energy.[1] It represents one potential step in the broad scheme of carbon capture and utilization.is a process that connects carbon capture with the production of useful chemicals and fuels. It uses electricity to convert captured carbon dioxide into different products, (see Figure 1) and the process becomes more sustainable when renewable electricity is used. Although this technology has received a lot of attention, it is still developing. Before large scale industrial use, challenges like product selectivity, energy efficiency, high current density, and long-term catalyst stability need must be addressed and solved.

The fundamental goal of this process is to complete the carbon cycle. Initially, CO_2 can capture from industrial emissions or other origin and then converted into valuable products instead of being discarded as a waste gas. The resulting products may include carbon monoxide, formate or formic acid, methanol, methane, ethylene, ethanol, propanol, and various chemical compounds. Carbon monoxide and formate are considered significant products because they can be produced with relatively good selectivity and have several industrial applications. The electrochemical conversion of CO_2 primarily occurs at the cathode of an electrochemical cell. Here, CO_2 gains electrons and typically reacts with protons sourced from water. Concurrently, an oxidation reaction happens at the anode to complete the electrical circuit. Thus, the entire process encompasses both reduction and oxidation reactions.[2]

Most commonly used metal for cathode catalysts for electrochemical CO_2 reduction into various products as follows:

Major Product	Common Cathode Catalyst
Carbon monoxide (CO)	Gold, Silver, Zinc
Formic acid (HCOOH)	Tin, Bismuth, Lead, Indium
Methanol (CH_3OH)	Copper based catalysts
Methane (CH_4)	Copper
C_2+products (ethylene, oxalate, ethanol)	Copper (for hydrocarbons), lead or mercury (for oxalate formation)

The following equations illustrate several important products obtained through CO_2 electroreduction in acidic or suitably buffered media. The actual dominant species and balanced half-reactions depend on the electrolyte pH and operating conditions.

Products	Cathodic Half-Reaction	Electrons Transferred
Carbon monoxide	$CO_2 + 2H^+ + 2e^- \rightarrow CO + H_2O$	2
Formic acid	$CO_2 + 2H^+ + 2e^- \rightarrow HCOOH$	2
Methanol	$CO_2 + 6H^+ + 6e^- \rightarrow CH_3OH + H_2O$	6
Methane	$CO_2 + 8H^+ + 8e^- \rightarrow CH_4 + 2H_2O$	8
Ethylene	$2CO_2 + 12H^+ + 12e^- \rightarrow C_2H_2 + 4\ H_2O$	12
Ethanol	$2CO_2 + 12H^+ + 12e^- \rightarrow C_2H_5OH + 3H_2O$	12

The process of electrochemically reducing CO_2 involves multiple complex steps due to the molecule's inherent stability, necessitating considerable energy for activation. Catalysts are utilized to lower these energy barriers and guide the reaction towards the formation of specific products by influencing selectivity. Initially, CO_2 is adsorbed onto the catalyst's surface, initiating a sequence of proton and electron transfers that create adsorbed intermediates. Key intermediates include *COOH (carboxyl intermediate) and *OCHO (formate intermediate), which are typically linked to the production of carbon monoxide and formate, respectively. The *COOH intermediate can undergo further reduction to form adsorbed *CO, which might either desorb as carbon monoxide or be further reduced to yield methane, methanol, and other hydrocarbons (see, Figure 2). Conversely, the *OCHO intermediate promote C–H bond formation and subsequent release of formate or formic acid, depending on the electrolyte environment. Additional transformations of adsorbed intermediates may result in the formation of multi-carbon (C_2+) products. The stability and reactivity of these intermediates, thus distribution of product are strongly influenced by factors such as catalyst composition and surface structure, applied potential, local pH, and solvent environment. Consequently, CO_2 electroreduction proceeds through interconnected reaction pathways that determine the efficiency and selectivity of fuel and chemical production. [3]

Adsorbed *CO is a key intermediate in CO_2 electroreduction, serving as a precursor for both carbon monoxide and a wide range of more reduced products. While *CO may desorb from the

catalyst surface as carbon monoxide, it can also remain adsorbed and undergo further proton- and electron-transfer reactions. On suitable catalyst surfaces, particularly copper-based materials, *CO intermediates can couple to form carbon-carbon (C −C) bonds, leading to the production of multicarbon (C_2+) compounds such as ethylene and ethanol. The efficiency and selectivity of these pathways are strongly influenced by catalyst surface structure, crystallographic orientation, electrode potential, local CO concentration, electrolyte composition, pH, proton availability, and reactant transport near the electrode. At the same time, the hydrogen evolution reaction competes with CO_2 reduction in aqueous electrolytes, making the choice of catalyst and electrolyte crucial for suppressing hydrogen formation and promoting the selective conversion of CO_2 into valuable carbon-based products.

A representative acidic-medium half-reaction is: $2H^+ + 2e^- \rightarrow H_{2(g)}$

Consequently, catalyst design aims not only to accelerate CO_2 reduction but also to suppress competing reactions. This can be achieved through the control of active sites, local pH, electrolyte composition, gas transport, and electrode wetting.

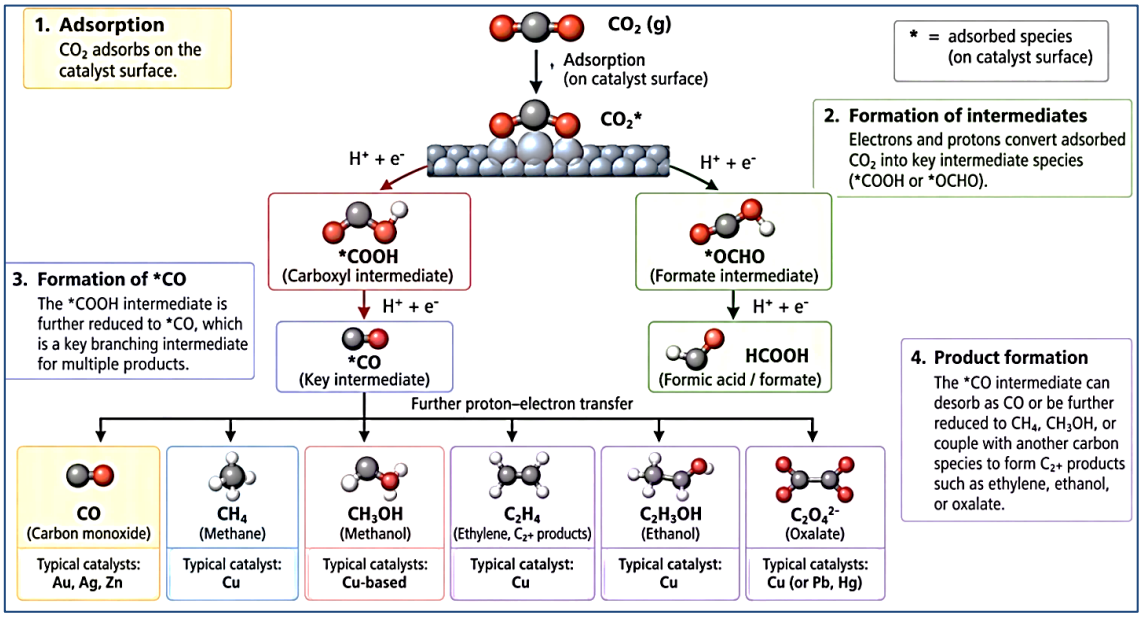


Figure 2: Schematic mechanism of electrochemical CO_2 reduction pathways leading to CO, formic acid, methane, methanol, and other C_2+ products through key surface intermediates

2. CO_2 Capture and Conversion Approaches in Electrochemical Systems

Electrochemical conversion of CO_2 can be categorized based on the method of carbon dioxide supply to the system and whether the stages of capture and conversion are conducted independently or combined. The selected method greatly impacts energy usage, process efficiency, carbon utilization, and the overall economic viability.

a) Conventional capture and conversion

Traditional systems initially capture CO_2 from industrial emissions or alternative sources, after which it undergoes separation, purification, compression, and is then transported to an

electrochemical reactor for conversion. This setup permits the separate optimization of the capture and conversion phases. Nonetheless, the inclusion of extra steps like solvent regeneration, CO_2 purification, compression, and transportation elevates the total energy requirements and complicates the process.

b) Integrated CO_2 capture and conversion

An alternative strategy combines CO_2 capture and electrochemical conversion within a single process. In this method, the capturing medium acts as the carbon source for electrochemical reduction. Removing intermediate steps can lower energy needs linked to CO_2 desorption, purification, compression, and transportation.

c) Direct utilization of bicarbonate and carbonate solutions

An encouraging integrated method utilizes bicarbonate-rich or carbonate-containing capture solutions directly within electrochemical reactors. Under appropriate operating conditions, carbon species in solution produce CO_2 at the cathode surface, where electrochemical reduction takes place. This strategy could streamline process operations and enhance overall energy efficiency by preventing total CO_2 recovery prior to conversion. Even with these benefits, obstacles persist, such as carbonate buildup, constraints in membrane transport, limited carbon usage, and rival side reactions that diminish product yield and energy efficiency.

d) Influence of CO_2 source and purity

Electrochemical conversion can utilize CO_2 obtained from industrial flue gases, biogas upgrading processes, direct air capture systems, or other carbon-containing streams. The composition of these sources varies considerably. Impurities such as sulfur compounds, nitrogen oxides, oxygen, and water vapor can adversely affect catalyst performance and reactor operation. Consequently, the required degree of purification depends on both the CO_2 source and the tolerance of the electrochemical conversion system.

e) Importance of reactor design

The effectiveness of any CO_2 conversion approach depends strongly on reactor architecture. Reactor design governs CO_2 transport to catalytic sites, ion migration, product removal, and continuous operation capability. Therefore, catalyst performance must always be evaluated together with the corresponding reactor configuration.

3. Materials and Components Used in Electrochemical CO_2 Conversion

A conventional electrochemical CO_2 conversion system has three main components: electrodes, an electrolyte, and electrolyzer. The cathode contains the catalyst where CO_2 is reduced. The anode supports the oxidation reaction, while the electrolyte allows ions to move through the system. The catalyst used at the cathode has a major effect on the reaction. Its composition and surface structure influence which reaction intermediates are formed and how strongly they interact with the catalyst surface. This ultimately determines which products are obtained. Metal

catalysts are widely used because they have good electrical conductivity and their surface properties can be controlled. Copper, indium, platinum, gold and silver etc. are commonly associated with the production of carbon monoxide and other C_2+ products.[4]

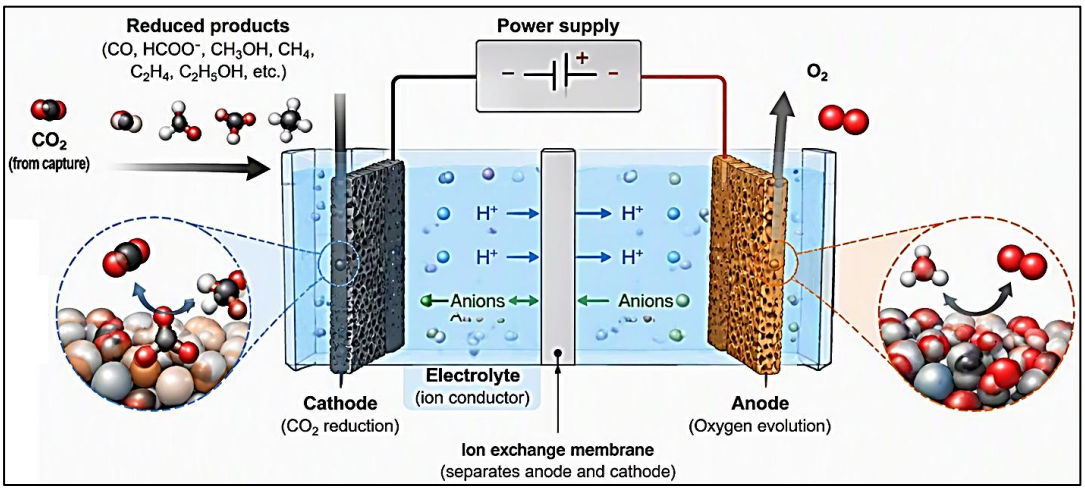


Figure 3: Schematic representation of an electrochemical CO_2 reduction system highlighting the roles of the cathode, electrolyte, anode, and catalyst

Gold has been widely studied because changes in particle size, surface structure, grain boundaries, and supporting materials can affect its ability to produce CO. Materials such as tin, bismuth, and indium are commonly studied for the production of formate or formic acid. Their performance can change depending on the size of the particles, their structure, and the material supporting the catalyst. Copper is one of the most important catalysts for producing products containing two or more carbon atoms. This is because copper can hold CO-related intermediates on its surface long enough for further reactions and carbon-carbon bond formation to occur. Researchers are studying different ways of improving copper catalysts by changing their composition, oxidation state, shape, surface structure, defects, and strain. Other types of catalysts are also being investigated. These include single-atom catalysts, molecular catalysts, and metal-organic frameworks. These materials can provide specific active sites and may use metal atoms more efficiently. Carbon-based materials and materials containing elements such as nitrogen can also be used as catalysts or supports and can be useful for producing carbon monoxide.

The electrolyte is another important part of the system. Water-based electrolytes are inexpensive and easy to use, but they have limited CO_2 solubility. Organic electrolytes can dissolve more CO_2 and provide a wider electrochemical operating range, but they may create problems related to toxicity, safety, and stability. Ionic liquids have also been studied because they can interact strongly with CO_2 and, in some cases, reduce unwanted hydrogen formation.

4. Comparison of Electrochemical Reactor Designs

Electrochemical CO_2 reduction can be performed in different reactor configurations. Each designed to improve reactant transport, catalyst utilization, product selectivity, and overall energy efficiency. Reactor architecture controls the delivery of CO_2 to the catalyst surface, ion

transport within the electrolyte, product removal, and the feasibility of continuous operation. As a result, reactor design plays a crucial role in determining the performance of electrochemical CO_2 conversion systems. One of the most common laboratory systems is the H-type cell.

a) H-Type Electrochemical Cells

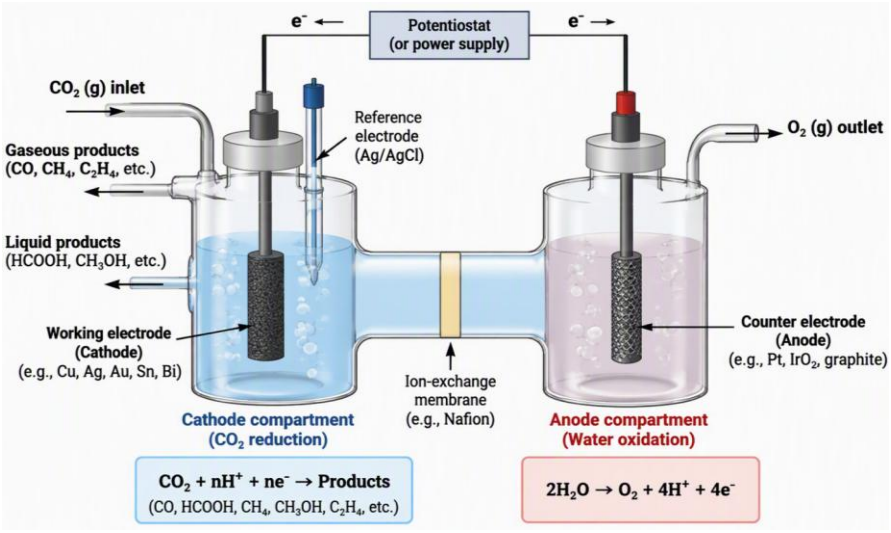


Figure 4: Schematic diagram of an H-type electrochemical cell used for CO_2 reduction, consisting of cathodic and anodic compartments separated by an ion-exchange membrane

CO_2 is reduced at the cathode, while water oxidation occurs at the anode. It generally consists of two separate chambers connected by an ion-conducting membrane or separator. One chamber contains the cathode, where CO_2 reduction takes place, while the other contains the anode, where the oxidation reaction occurs. The cathode is usually immersed in an electrolyte containing dissolved CO_2. When an appropriate potential is applied, electrons are transferred to CO_2 molecules at the catalyst surface. Depending on the catalyst and reaction conditions, different products such as carbon monoxide, formate, methane, ethylene, ethanol, or other compounds can be produced. H-type cells are especially useful for fundamental research. They allow researchers to study the behaviour of catalysts under controlled conditions and compare the effects of different electrode materials, electrolytes, pH values, applied potentials, investigating reaction mechanism and identifying intermediate in CO_2 reduction. H-type electrochemical cells suffer from low CO_2 mass transfer due to the limited solubility of CO_2 in aqueous electrolytes, resulting in low current densities and reduced reaction rates. They are therefore mainly used for laboratory-scale studies and catalyst evaluation rather than industrial-scale CO_2 reduction.

b) Flow Cells and Gas Diffusion Electrodes

To overcome the limitations of H-type cells, researchers have developed flow cells and gas diffusion electrode systems. In these reactors, CO_2 can be supplied more directly to the catalyst through a gas channel. A gas diffusion electrode, or GDE, contains a porous structure that allows gaseous CO_2 to travel through the electrode and reach the catalyst layer. The use of a gas diffusion electrode greatly improves the supply of CO_2 compared with systems where CO_2 must

first dissolve in a large volume of liquid electrolyte. This can significantly increase the amount of CO_2 available at the catalyst surface. As a result, much higher current densities can be achieved. Flow cells also allow the electrolyte and gaseous reactants to move continuously through the reactor. This provides better control over the supply of reactants and the removal of products. The continuous flow arrangement can also reduce the accumulation of products near the electrode surface.

c) Membrane Electrode Assemblies

Another important reactor technology is the membrane electrode assembly, commonly known as an MEA. MEAs are widely used in electrochemical and fuel-cell technologies and are increasingly being studied for CO_2 conversion. In an MEA, the cathode, membrane, and anode are placed very close together. The membrane separates the two electrodes while allowing selected ions to move between them. Because the components are closely integrated, the distance through which ions and reactants must travel is reduced.

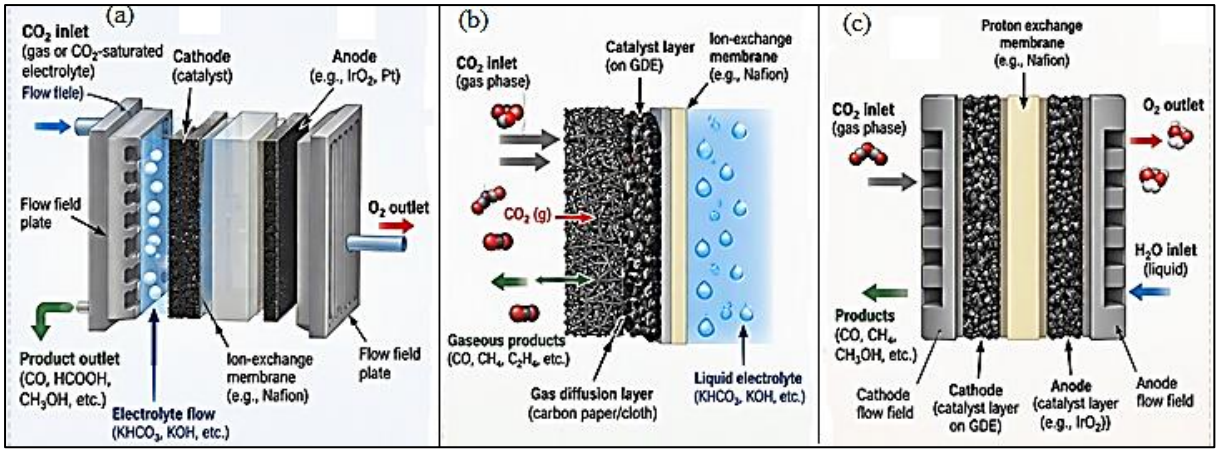


Figure 5: Schematic diagram of Flow cell (a), Gas Diffusion electrode cell (b) and Membrane electrode Assembly (c)

5. Classification Based on Products

Electrochemical CO_2 conversion can also be classified according to the products formed in the electrochemical reduction process. The products can broadly be divided into one-carbon products, commonly called C_1 products, and products containing two or more carbon atoms, known as C_2+ products. C_1 products contain a single carbon atom, important examples includes carbon monoxide, formate, methane, and methanol. Carbon monoxide is particularly important because it can be used as a chemical feedstock and can also be combined with hydrogen to produce synthesis gas and other chemicals. Formate and formic acid are useful in chemical manufacturing and are also being studied for applications related to hydrogen storage and fuel cells. Methane is a hydrocarbon fuel and can be produced through a series of proton-coupled electron-transfer steps. Methanol is another important product because it is widely used as a chemical feedstock, solvent, and fuel. However, producing these products selectively requires careful control of the catalyst and reaction conditions (see Figure 2).

C_2+ products contain two or more carbon atoms; examples include ethylene, ethanol, acetate, propanol, and other multicarbon compounds. These products are particularly interesting because many of them have applications as fuels or chemical feedstocks. The formation of C_2+ products is generally more difficult than the formation of many C_1 products. This is because the reaction must involve the formation of a carbon-carbon bond. In the case of copper-based catalysts, for example, carbon-containing intermediates formed during CO_2 reduction can interact with one another or with other surface intermediates. These reactions can lead to the formation of products containing two or more carbon atoms. The selectivity toward a particular product depends on many factors, including the catalyst composition, surface structure, electrolyte, pH, temperature, applied potential, CO_2 concentration, and local reaction environment. Small changes in these conditions can sometimes cause significant changes in the products formed.

a) Carbon Monoxide and Formate Production

Among the different products obtained through electrochemical CO_2 conversion, carbon monoxide and formate are commonly studied because they can be produced with relatively high selectivity using suitable catalysts. Carbon monoxide production generally involves a two-electron reduction of CO_2. (see Figure 2) Catalysts based on metals such as silver and gold can show good activity toward CO formation. The produced CO can either be collected as a product or used as an intermediate for further chemical conversion. Formate production also involves a relatively simple reduction pathway. Tin-, bismuth-, and indium-based catalysts have been widely investigated for producing formate or formic acid. Depending on the electrolyte and operating conditions, the product may remain in solution in the form of formate ions or may be recovered as formic acid after further processing. These reactions are attractive because CO and formate have established industrial uses. However, the economic value of the overall process depends on factors such as electricity cost, CO2 source, product concentration, separation requirements, catalyst lifetime, and energy efficiency.

b) C_2+ Product Formation

The production of C_2+ compounds is one of the most active areas of research in electrochemical CO_2 conversion. These products include ethylene, ethanol, acetate, propanol, and other oxygenated hydrocarbons. Copper is particularly important in this area because it is one of the few catalyst materials that can produce significant amounts of multicarbon products under suitable conditions. Researchers have developed different copper structures, including nanoparticles, nanocubes, porous copper, oxide-derived copper, and copper-based alloys, to control the reaction pathway. The formation of C_2+ products requires carbon-carbon coupling between reaction intermediates. This makes the process more complex than the production of many C_1 compounds. The local environment near the catalyst surface, including pH, CO concentration, water availability, and the structure of the catalyst surface, can influence whether C_1 or C_2+ products are formed. Ethylene is one of the important C_2 products because it is a major

industrial chemical used in the production of plastics and other materials. Ethanol is also of interest because it can be used as a fuel, solvent, and chemical feedstock. Acetate and propanol have additional applications in chemical and biological processes. Although C_2+ products have significant potential value, their production often involves several competing reactions. Hydrogen evolution can occur at the same time as CO_2 reduction, and several carbon-containing products may be formed simultaneously. Therefore, improving selectivity remains a major research objective.

6. Applications of Electrochemical CO_2 Conversion

One of the most important applications of electrochemical CO_2 conversion is the production of useful chemical intermediates. Carbon monoxide is particularly important because it can be used in syngas production and as a starting material for making other chemicals. Formate and formic acid are also important products because they have applications in chemical industries and have been considered as possible energy carriers. Another possible application is the production of renewable fuels. Products such as methanol, methane, ethylene, ethanol, and propanol can be used as fuels or as raw materials for chemical production. Liquid products are especially interesting because they can store energy in a relatively compact form and may be easier to transport and store than gaseous products.

Electrochemical CO_2 conversion can also be used as part of industrial carbon management. For example, CO_2 from industrial facilities could potentially be captured and converted at or near the same site. This would reduce the need to transport large amounts of CO_2. However, the quality of the captured CO_2 and the presence of impurities must be considered because they can affect the catalyst and the overall process. Another developing area is the production of higher-value chemicals. Instead of converting CO_2 only into simple fuels, researchers are studying ways to combine CO_2-derived intermediates with other molecules. These reactions can produce compounds containing carbon-nitrogen or carbon-oxygen bonds and may be useful for producing specialty chemicals.

7. Limitations and Future Perspective of Electrochemical CO_2 Conversion

Despite significant advances in electrochemical CO_2 conversion, several challenges continue to hinder its large-scale deployment. A major limitation is the high energy demand (high cost of electricity) associated with activating the highly stable CO_2 molecule, particularly for the production of multi-carbon fuels and chemicals. Product selectivity remains difficult to achieve because multiple reaction pathways often operate simultaneously, leading to mixtures of products and increasing downstream separation costs.[5] The hydrogen evolution reaction (HER) competes directly with CO_2 reduction in aqueous systems, lowering carbon utilization efficiency and reducing the yield of desired products. In addition, the low solubility and slow mass transport of CO_2 in conventional electrolytes limit reaction rates and achievable current densities. Long-term operation is further challenged by catalyst deactivation, electrode flooding, membrane

degradation, and carbonate formation, all of which can decrease system performance and durability. The presence of impurities in industrial CO_2 streams may also adversely affect catalyst activity and membrane stability, necessitating additional gas purification steps. Finally, significant engineering challenges remain in scaling laboratory-scale systems to industrial operation while maintaining efficiency, stability, and economic viability.

Future Perspectives

Future developments in electrochemical CO_2 conversion are expected to focus on highly selective and durable catalysts, advanced electrolyzer configurations, and improved membrane technologies capable of operating efficiently at industrially relevant current densities. Particular attention is being given to the production of carbon monoxide and formate because of their relatively high selectivity and established industrial applications. Advances in gas-diffusion electrodes, membrane-electrode assemblies, and integrated carbon capture and conversion systems are expected to improve reaction rates, carbon utilization, and overall energy efficiency.

A promising future approach involves the direct integration of carbon capture and electrochemical conversion technologies. In such systems, CO_2 emitted from power plants, cement factories, steel industries, and other industrial sources could be captured using dedicated adsorption or absorption units and fed directly into electrochemical reactors. The electricity required for conversion may be supplied by renewable energy sources such as solar photovoltaic panels. Excess solar electricity generated during the daytime can be stored in batteries or inverter-based energy storage systems and subsequently used to drive CO_2 conversion during periods without sunlight. This integrated approach would enable continuous operation while reducing dependence on fossil-fuel-derived electricity.

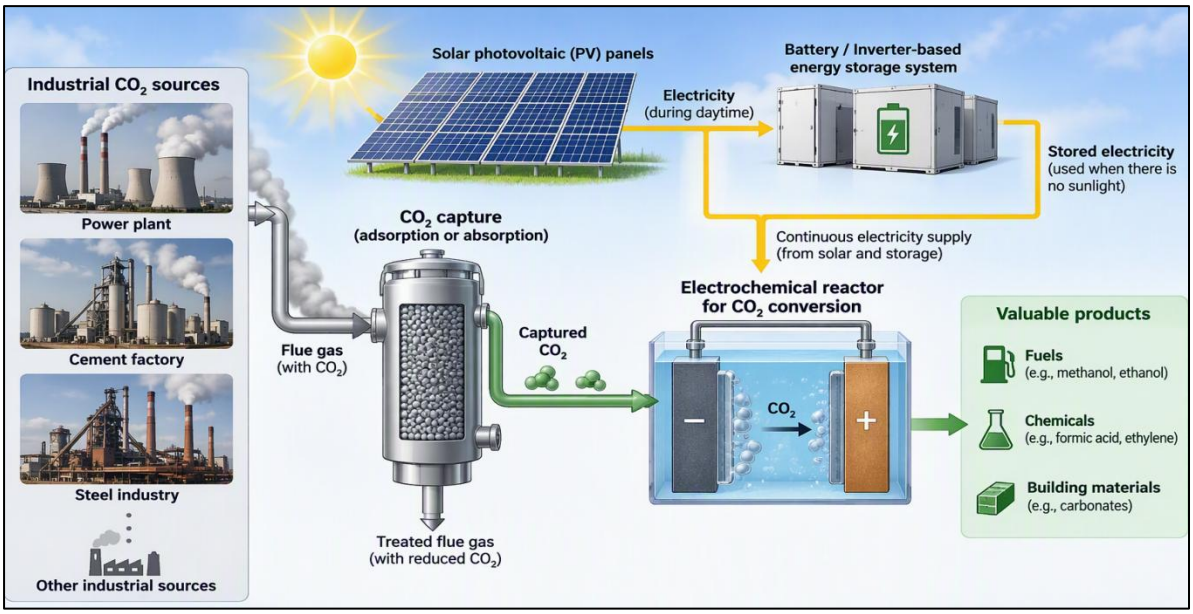


Figure 6: Conceptual framework for coupling industrial CO_2 capture with solar-powered electrochemical conversion

Future research is also expected to focus on selective product formation through rational catalyst design, optimized reactor operation, and improved electrolyte engineering. By carefully tailoring catalyst composition and reaction conditions, it may become possible to preferentially produce a single desired product, thereby minimizing downstream separation costs. Where multiple products are formed, advances in separation technologies will be required to efficiently recover individual chemicals and fuels. Standardized performance evaluation, together with techno-economic analysis and life-cycle assessment, will be essential for identifying commercially viable pathways. Ultimately, the combination of carbon capture, renewable electricity, energy storage, and efficient electrochemical conversion offers a promising route for reducing CO_2 emissions while simultaneously producing valuable fuels and chemical feedstocks, thereby contributing to a sustainable circular carbon economy.

Conclusion

In conclusion electrochemical CO_2 conversion is an emerging technology that provides a possible link between carbon capture and the production of useful chemicals and fuels. Considerable progress has been made in understanding CO_2 reduction reactions, developing catalysts, and designing more efficient electrochemical reactors. Different catalysts can produce different products, ranging from carbon monoxide and formate to methanol, methane, ethylene, ethanol, and other hydrocarbons. The technology has several potential advantages, particularly when renewable electricity is used and when CO_2 capture and conversion are integrated into the same process. However, important challenges remain, including energy efficiency, product selectivity, catalyst stability, high current density, product separation, and carbon losses.

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A SOLVENT-FREE, MICROWAVE-ASSISTED GREEN PROTOCOL FOR SYNTHESIZING 1,2-DISUBSTITUTED BENZIMIDAZOLES

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Abstract

An environmentally benign and operationally simple microwave-assisted protocol has been developed for the efficient synthesis of 1,2-disubstituted benzimidazoles under solvent-free conditions. This process uses 1-fluoro-2-nitrobenzene, various primary aromatic amines, and aldehydes in the presence of sodium dithionite to afford the target molecules in excellent yields within just 30 minutes at 60 °C. Unlike earlier conventional heating methods, this green approach eliminates the use of toxic solvents, avoids chromatographic purification, and significantly reduces reaction time and energy consumption. All products synthesized are previously reported in the literature; however, they have been fully characterized using both ^{1}H and ^{13}C NMR spectroscopy. This method represents a sustainable and scalable alternative for the synthesis of known benzimidazole derivatives.

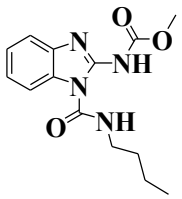
Keywords: Microwave-Assisted Synthesis, Benzimidazoles, Solvent-Free, Green Chemistry, Disubstituted Benzimidazoles.

1. Introduction

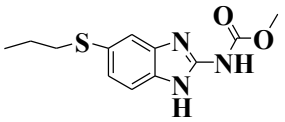
Naturally occurring and synthetically derived substituted benzimidazoles display a broad spectrum of biological activities, making them highly appealing to organic chemists[1]. These compounds serve as powerful inhibitors of hepatitis C virus NS5B polymerase and act as selective antagonists[2] of the angiotensin II type 1 receptor. Selectively substituted benzimidazoles are widely used as pharmaceutical agents—including well-known anthelmintics like albendazole, fenbendazole, oxfenbendazole, thiabendazole, and mebendazole, as well as proton pump inhibitors such as omeprazole, lansoprazole, and pantoprazole—across both human and veterinary medicine (Fig. 1) [3]. Beyond therapeutics, benzimidazole-based molecules have garnered significant interest for their applications in fungicides, enzyme inhibitors, dyes, polymers, chemosensors, and fluorescent probes[4]. This wide-ranging utility underscores the importance of developing efficient synthetic routes to tailor-made 1,2-disubstituted benzimidazole derivatives.

Multiple synthetic routes have been developed for 1,2-disubstituted benzimidazole derivatives, most notably: N-alkylation of 2-substituted benzimidazoles under strong basic conditions[5],

reductive cyclization of N-substituted o-aminoanilines with aldehydes[6], and the condensation of N-substituted o-phenylenediamines with the sodium salt of hydroxybenzylsulfonic acid[7].



Albendazole
antiprotozoal agent

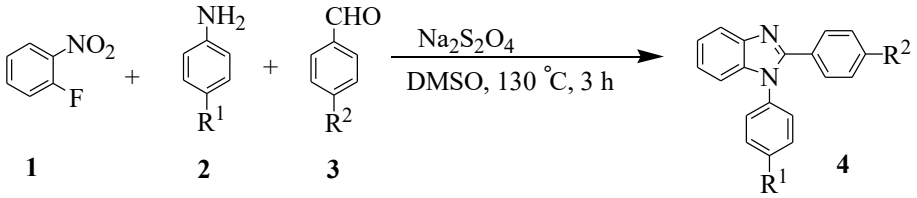


Benomyl
fungicide

Figure 1: Drug molecules containing benzimidazole moiety

Among the various strategies for synthesizing 1,2-disubstituted benzimidazoles, the most widely adopted approach involves the acid-catalyzed condensation of N-substituted o-phenylenediamines with aromatic aldehydes[8]. Numerous catalysts have been explored to facilitate this transformation. Although these methods often yield satisfactory results, they frequently suffer from limited control over regioisomeric selectivity due to the competitive formation of both 1,2- and 2-substituted benzimidazole isomers. Furthermore, many of the reported protocols involve harsh reaction conditions, expensive and environmentally hazardous metal-based catalysts, extended reaction times, and limited availability of starting materials. Consequently, the development of green, efficient, and regioselective synthetic methodologies for direct access to 1,2-disubstituted benzimidazoles remains a significant challenge and a focal point of ongoing research.

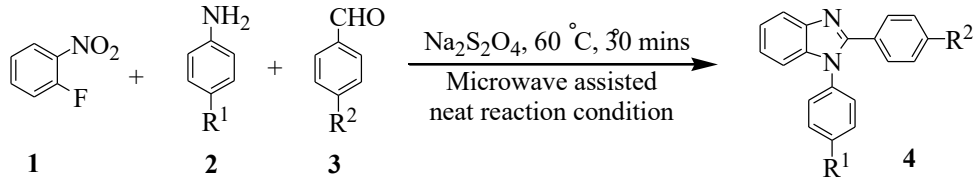
Previous work



1 **2** **3** **4**

Puer product after column chromatography using silica gel, ethylacetate/petroleum ether

This work



1 **2** **3** **4**

Puer product after filtration and recrystallization using aqueous ethanol

Scheme 1: Green strategy towards 1,2-disubstituted benzimidazoles.

In our earlier work, we reported a one-pot, sequential, metal-free synthesis of 1,2-disubstituted benzimidazoles (Scheme 1)[9]. The protocol encompasses the coupling of a primary amine with 1-

fluoro-2-nitrobenzene, followed by sodium dithionite-mediated reduction of the resulting nitroarene, and subsequent cyclization of the in-situ formed diamine with an aldehyde. This strategy offers notable advantages, including excellent regioisomeric control, metal-free and near-neutral conditions, and elimination of intermediate isolations. However, despite its strengths, the method is limited by key drawbacks: the use of non-green solvents such as DMSO, a labor-intensive work-up and purification process that relies on silica gel chromatography and conventional solvents like ethyl acetate and petroleum ether, and the requirement for prolonged reaction times of at least 3 hours. Moreover, the reaction demands high temperatures, requiring heating up to 130 °C to achieve optimal conversion.

2. Materials and Method

The central advancement presented in this study lies in the development of a green, microwave-assisted protocol for the efficient synthesis of 1,2-disubstituted benzimidazole derivatives (4). Utilizing 1-fluoro-2-nitrobenzene (1), various primary amines (2), and aldehydes (3) in the presence of sodium dithionite under solvent-free conditions (Scheme 1), this method addresses critical limitations of conventional routes. Unlike earlier approaches, it avoids non-green solvents, reduces energy consumption through microwave irradiation, and eliminates the need for tedious silica gel column chromatography and hazardous solvents such as ethyl acetate and petroleum ether during work-up. Most importantly, this protocol operates at a significantly reduced temperature (60 °C) and achieves complete conversion in just 30 minutes, making it a time-efficient, environmentally benign alternative. These combined advantages align with current green chemistry principles and enhance the sustainability and scalability of benzimidazole synthesis.

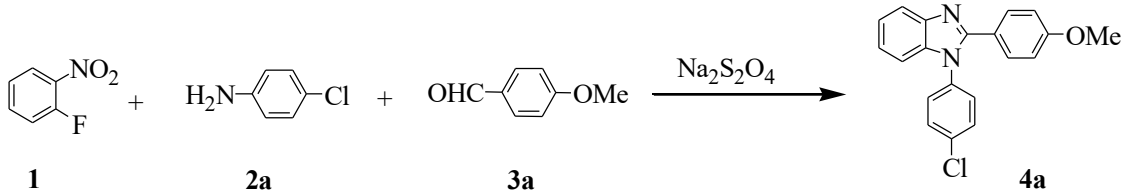
All experiments were conducted under ambient atmospheric conditions using flame-dried reaction vessels. Prior to use, all reagents were carefully dried and purified through distillation. Following extraction, the organic layers were concentrated by evaporation under reduced pressure. Melting points were determined as recorded, without any correction.

3. Results and Discussion

With the aim of establishing an environmentally friendly and practical protocol, we initially investigated the synthesis of 1,2-disubstituted benzimidazoles via the coupling of 1-fluoro-2-nitrobenzene (1), p-chloroaniline (2a), and p-methoxybenzaldehyde (3a) in aqueous medium (Table 1). However, no product (4a) formation was observed, likely due to the poor solubility of the substrates (Table 1, Entry 1). Subsequently, alcohols such as methanol and ethanol were employed as greener alternatives to hazardous organic solvents, but the desired benzimidazole derivative (4a) was obtained in only 5–7% yield, along with unreacted starting materials (Entries 2 and 3). These unsatisfactory results prompted us to attempt the reaction under solvent-free conditions. Prior to reaction, the solid and liquid components were thoroughly mixed using a

mortar and pestle to ensure uniform distribution and intimate contact among the reactants under neat conditions. While this method is operationally simple and environmentally benign, the product was obtained in low yield even after 3 hours (Entry 4). Encouraged by the effect of temperature, we increased the reaction temperature to 100 °C, which led to a notable improvement in yield (Entry 5). However, reducing the reaction time resulted in a corresponding decrease in yield. Ultimately, the best result was achieved when the neat mixture of reactants was subjected to microwave (MW) irradiation at 60 °C for 30 mins, affording the product in 77% yield (Entry 7). In all cases, the reaction progress was monitored by thin-layer chromatography (TLC), and the crude product was extracted with ethyl acetate and washed with water, followed by purification through crystallization using aqueous ethanol. The structure of the purified product was confirmed by comparison of its melting point, ^{1}H NMR and ^{13}C NMR spectrum with previously reported data.

Table 1: Effect of Reaction Conditions on the Synthesis of Benzimidazole Derivative 4a[a]



1 **2a** **3a** **4a**

Entry	Solvent	Temp. (°C)	Conc. (M)[b]	Time (h)	Yield (%)[c]
1	H2O	100	0.7	5	0
2	MeOH	64	0.7	5	5
3	EtOH	78	0.7	5	7
4	Nil	r.t.	–	3	14
5	Nil	100	–	5	37
6	Nil	100	–	3	24
7	**Nil**	**60**	–	**30 mins**	**87[d]**

[a]1-fluoro-2-nitrobenzene-amine-aldehyde-sodium dithionite in ratio 2:2.1:2.1:2.3

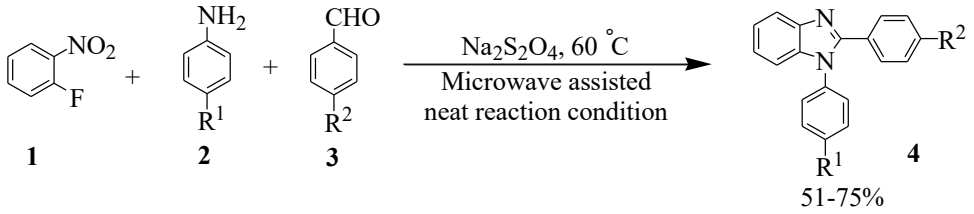
[b]Starting materials (1-fluoro-2-nitrobenzene, amine and aldehyde) concentration in solvents

[c]Isolated yields

[d]Under MW irradiation

Encouraged by the success of the microwave-assisted, solvent-free protocol, we extended this method to a variety of aldehydes and primary amines to explore its generality (Table 2). In each case, the corresponding 1,2-disubstituted benzimidazole derivatives were obtained in good yields. The identity of the product was confirmed by comparison with authentic sample[9a,10]. The melting point,^{1}HNMR and ^{13}C NMR spectra were in full agreement with reported data.

Table 2: 1,2-Disubstituted benzimidazoles 4 synthesis under optimized conditions



Entry	R^1	R^2	Yield[a] (%)
a	Cl	OMe	77
b	Cl	OH	92
c	Cl	NMe_2	87
d	Cl	F	87
e	CH_3	F	75
f	OMe	F	90

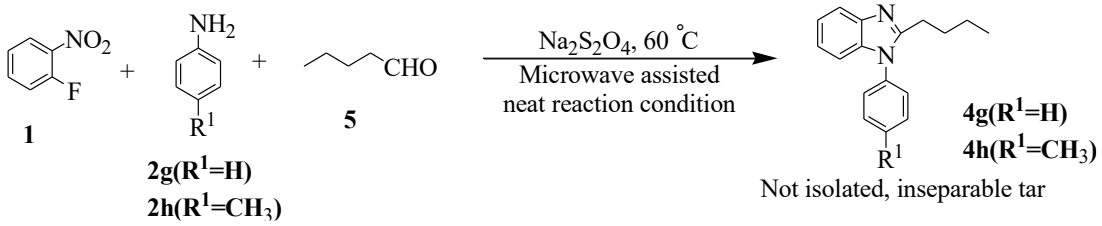
[a]Yields isolated.

Importantly, this method represents a clear improvement over our previous protocol. It avoids the use of DMSO and chromatographic solvents like ethyl acetate and petroleum ether. It also reduces the reaction temperature from 130 °C to 60 °C and the time from 3 hours to just 30 minutes, resulting in substantial energy savings (Table 3).

Table 3: Comparison of Conventional vs Microwave Method

Feature	Conventional Method (2013)	This Work (2025)
Heating Method	Conventional oil bath	Microwave irradiation
Reaction Temperature	130 °C	60 °C
Reaction Time	≥3 h	30 min
Solvent Used	DMSO	None
Work-Up	Column chromatography	Recrystallization
Energy Consumption	High	Low

Following the successful synthesis of a series of 1,2-disubstituted benzimidazoles bearing aromatic substituents, we sought to extend the same substitution/reduction/cyclization strategy to their aliphatic counterparts (Scheme 2). While the green work-up and separation process proved effective for aromatic substrates, it failed when applied to aliphatic aldehydes, leading to the formation of inseparable tar-like mixtures. In these cases, isolation of the pure products was not feasible; however, mass spectrometric analysis of the crude reaction mixtures confirmed the presence of the target benzimidazole derivatives.



Scheme 2: Synthetic Strategy for Aliphatic-Substituted Benzimidazoles

3. Experimental

1. General

All reagents and solvents were obtained commercially and used without further purification unless otherwise stated. Sodium dithionite was purchased from Aldrich. Microwave-assisted reactions were performed using a multimode microwave chemical reactor (OLT CR-2, Xiamen Ollital Technology Co., Ltd., China). Reactions were conducted under an open atmosphere in flame-dried glassware. Melting points are uncorrected.

Typical synthetic protocol for 1,2-disubstituted benzimidazoles. 1-Fluoro-2-nitrobenzene **1** (2.0 mmol), the appropriate amine **2** (2.1 mmol), sodium dithionite (2.3 mmol), and the corresponding aldehyde **3** (2.1 mmol) were combined and thoroughly ground using a mortar and pestle under solvent-free (neat) conditions to ensure uniform mixing and intimate contact of the reactants. The resulting homogeneous blend was transferred into a sealed microwave-compatible glass reaction vessel and subjected to microwave irradiation at 60 °C. The temperature was precisely regulated using the reactor's built-in PID-controlled thermocouple system. The course of the reaction was monitored by thin-layer chromatography (TLC). Upon completion, the reaction mixture was treated with water (20 mL) and extracted with ethyl acetate (20 mL). The organic phase was subsequently washed with water (3 × 20 mL) followed by brine (5 mL), dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The crude residue was purified by recrystallization from aqueous ethanol to afford the desired product **4** in pure form. All synthesized compounds were confirmed by comparison with literature-reported data.

2-(4-Methoxyphenyl)-1-(4-chlorophenyl)-1H-benzo[d]imidazole (4a). A mixture of 1-fluoro-2-nitrobenzene **1** (282 mg, 2.0 mmol), *p*-chloroaniline **2a** (267 mg, 2.1 mmol), sodium dithionite (400 mg, 2.3 mmol), and 4-methoxybenzaldehyde **3a** (285 mg, 2.1 mmol) was treated following the general procedure to furnish a yellow solid, benzimidazole **4a** (514 mg, 77%). **MP:** 168 °C (Lit. 169–170 °C); **^{1}H NMR (300 MHz, $CDCl_3$):** δ 7.86 (d, 1H, J = 8.1 Hz), 7.48 (dd, 4H, J = 9.0, 3.0 Hz), 7.30–7.18 (m, 5H), 6.84 (d, 2H, J = 8.7 Hz), 3.83 (s, 3H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ 160.0, 151.6, 142.2, 136.7, 135.2, 133.8, 130.5, 129.5, 128.2, 122.6, 122.4, 121.4, 119.2, 113.2, 109.5, 54.4;

2-(4-Hydroxyphenyl)-1-(4-chlorophenyl)-1H-benzo[d]imidazole (4b). A mixture of 1-fluoro-2-nitrobenzene **1** (282 mg, 2.0 mmol), *p*-chloroaniline**2b** (267 mg, 2.1 mmol), sodium dithionite

(400 mg, 2.3 mmol), and 4-hydroxybenzaldehyde **3b** (256 mg, 2.1 mmol) was treated following the general procedure to furnish a white solid, benzimidazole **4b** (588 mg, 92%). **MP:** >200 °C (Lit. >300 °C);

2-(4-(*N,N*-Dimethylamino)phenyl)-1-(4-chlorophenyl)-1H-benzo[d]imidazole (4c). A mixture of 1-fluoro-2-nitrobenzene **1** (282 mg, 2.0 mmol), *p*-chloroaniline **2c** (267 mg, 2.1 mmol), sodium dithionite (400 mg, 2.3 mmol), and *p*-dimethylaminobenzaldehyde **3c** (313 mg, 2.1 mmol) was treated following the general procedure to furnish a white solid, benzimidazole **4c** (604 mg, 87%). **MP:** 164 °C (Lit. 164-166 °C);

2-(4-Fluorophenyl)-1-(4-chlorophenyl)-1H-benzo[d]imidazole (4d). A mixture of 1-fluoro-2-nitrobenzene **1** (282 mg, 2.0 mmol), *p*-chloroaniline**2d** (267 mg, 2.1 mmol), sodium dithionite (400 mg, 2.3 mmol), and 4-fluorobenzaldehyde **3d** (261 mg, 2.1 mmol) was treated following the general procedure to furnish a white solid, benzimidazole **4d** (562 mg, 87%). **MP:** 168 °C (Lit. 166–168 °C);

1-(p-Tolyl)-2-(4-fluorophenyl)-1H-benzo[d]imidazole (4e). A mixture of 1-fluoro-2-nitrobenzene **1** (282 mg, 2.0 mmol), *p*-tolylamine**2e** (225 mg, 2.1 mmol), sodium dithionite (400 mg, 2.3 mmol), and 4-fluorobenzaldehyde **3e** (290 mg, 2.1 mmol) was treated following the general procedure to furnish a white solid, benzimidazole **4e** (454 mg, 75%). **MP:** 119 °C (Lit. 119–121 °C);

1-(4-Methoxyphenyl)-2-(4-fluorophenyl)-1H-benzo[d]imidazole (4f). A mixture of 1-fluoro-2-nitrobenzene **1** (282 mg, 2.0 mmol), *p*-methoxyaniline**2f** (258 mg, 2.1 mmol), sodium dithionite (400 mg, 2.3 mmol), and 4-fluorobenzaldehyde **3f** (261 mg, 2.1 mmol) was treated following the general procedure to furnish a white solid, benzimidazole **4f** (572 mg, 90%). **MP:** 119 °C (Lit. 118–120 °C);

Conclusion

A solvent-free, microwave-assisted protocol has been developed for the efficient synthesis of 1,2-disubstituted benzimidazoles. This method offers a green alternative to conventional approaches by significantly reducing reaction time, lowering reaction temperature, and eliminating the need for toxic solvents and chromatographic purification. The target compounds were obtained in excellent yields and fully characterized using melting point, ^{1}H NMR, and ^{13}C NMR spectroscopy. A comparative evaluation confirms the enhanced sustainability and practicality of this method over previously reported procedures. Despite the known nature of the products, the improved operational simplicity, energy efficiency, and environmental benefits underscore the utility of this approach. This work reinforces the value of microwave irradiation in promoting greener synthetic methodologies and may serve as a useful reference for future developments in sustainable heterocyclic chemistry.

Acknowledgment

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AN ANALYTICAL STUDY OF CHAIN OF CUSTODY IN DF

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Abstract
Chain of Custody (CoC) plays a role in digital forensics (DF) to maintain integrity, reliability, correctness, authentication in digital evidence. CoC works on verification that evidence which are collected, transformed, analyzed cannot be changed or altered at all phases. It is a process which handles evidence that are used in court and for analysis. It is important because ensures evidence is reliable, secure, legally valid throughout the investigation. The main aim of Chain of Custody (CoC) is only accessible person can access evidence and unnecessary person do not access the evidence and cannot change or altered evidence which are collected, transformed into informative evidence, used for analysis and presented in the court. Chain of Custody (CoC) refers to systematic process from which evidence is collected and presented in court for analysis. Its primary objective is maintaining the evidence in correct way like collect data, maintain it, analysis for create valid evidence for presented in court. This study also highlighting the importance of CoC which helps in maintaining legal evidence for judicial decisions. CoC also helps how to maintain and secure evidence. CoC also includes how, when, where from the evidence is collected.

Keywords: Chain of Custody (CoC), Evidences, Integrity and Authenticity, Digital Forensics (DF).

1. Introduction

CoC plays important role in DF because its help how the evidence is created, collected, transferred, analysed and presented in court. This also helps evidence is authentic, reliable, correct during presented in the court. Each person who handled evidence is also required to testify the evidence for the correctness, reliability and authentic of the evidence.[1] It is also important for legal investigation in which the evidence is handled, recorded, collected it properly. It plays a crucial role for maintaining integrity and authenticity of the evidence. Improper evidence and documentation create rejection of evidence. It also involves proper recording of who collected, handled, transferred, and stored the evidence. CoC helps to ensure the evidence is reliable, correct, legally acceptable and also support correct and fair decisions. CoC refers to the process of validating how any kind of evidence has been gathered, tracked, and protected on its way to a court of law. It guarantees that the data presented is “as originally acquired and has not been tampered with and is authentic prior to admission into evidence.”[2] This study helps to examine the importance, methods and challenges of CoC.

The issues that are faced by the person who collected the evidence is improper documentation, evidence tampering, loss of evidence, contamination, break in chain, human error, lack of training means do not follow proper procedures. CoC is important because evidence remains safe, authentic, unchangeable throughout the investigation. It also provides a clear and continuous record of the evidence that how, where the evidence is collected, transferred, stored which maintains integrity. By preventing from improper documentation, evidence tampering, loss of evidence, contamination, break in chain, human error and lack of training makes evidence reliable and trustworthy. By proper maintaining of Chain of Custody (CoC) make fair and correct decision in court.

The aim of research of CoC is dealing with how data is collected for the evidence. For which how data is collected, how data transferred, how analysis working for the collection of evidence. For find and prove in CoC is how evidence is collected, transferred, stored, analysis and how it presented in particular form in court. How to check the evidence is correct or trustworthy. To learn what step we perform after each stage when we collect the data. The dataset has been taken from online:

https://www.kaggle.com/datasets/esayasmelaku/deepfake-detection [3]

This study is useful for cybersecurity and forensics because the main purpose of CoC is investigation of documents and evidence is correct, trustworthy, reliable or not. It also helps investigators of forensics and cybersecurity in real life because Chain of Custody (CoC) helps the investigators how the evidence is collected, transferred and analysis and also helps which step performs one after another during investigation.

2. Literature Review

Literature review focuses on previous research of Chain of Custody (CoC). Many different authors classify the evidence integrity, accuracy, maintainability and authentication but still never focuses on how evidence is collected, why we need evidence, when did evidence is created, when we collected evidence how we know the collected evidence is correct. In this research paper we focus on what is CoC, why we need it, what steps perform when we collect evidence, when did evidence is created. CoC is a means by which inputs, outputs, and associated attributes are transferred, monitored and controlled as they move forward through each step in the supply chain[3]. Traceability is capability to monitor and confirm the origin and destination of movement of a material by the use of specific steps of production, processing and distribution.[3] A set of production, material and product characteristics that the CoC is designed to maintain by ISO.[3] Previous study focuses on Chain of Custody (CoC) used different methods to measure handling and tracking of evidence. There are three different types of studies such qualitative, quantitative and comparative methods of research.

Many authors use qualitative approach where case studies is analyzed where they analysed case study of criminal investigation to understand from where evidence was collected, documented like accuracy, maintainability of evidence and how it preserved. This qualitative method focuses on real world scenario to identify errors and for best practice.

Many of them uses quantitative method of research where experiments and simulations to evaluate the different evidence tracking system. Many of them uses comparative approach where traditional manual documentation compared with modern digital system. The result of comparative approach is more efficient and reduce human errors whereas manual documentation make mistakes like human misunderstands called human errors. It is widely used due to its simplicity and low cost.

Different researchers used different methods that provide valuable information but each of them has different strengths and limitations also while qualitative approach is best method of research because it provides detailed understanding of investigation.

The purpose of these three approaches is to answer research questions where we test and build new theories. They all required structured data collection, analysis and interpretation to achieve validity and readability. Their aim is to build relationships, trends and pattern.

Table 1: Comparison between Qualitative, Quantitative and Comparative approaches

Parameters	Qualitative Approach	Quantitative Approach	Comparative Approach
Purpose	It understands the concepts, experiences or meaning	It understands variables and test hypotheses	It compares two or more methods, groups or system.
Data types	Text, images	Numbers	Both (text, numbers)
Focuses	It understanding meaning	It measures and testing	It compares of system and groups
Methods	Case studies	Surveys, experiments and structured data collection	Cross case analysis
Analysis	Content analysis	Statistical techniques like mean, correlation and regression	Identify patterns, advantages and limitations

3. Research Gaps

Despite the growing research on DF and the chain of custody, several important gaps remain. Most studies focus mainly on technological solutions, such as blockchain, smart contracts, or automated evidence management systems. While these approaches improve security, transparency, and auditability, there is limited research on practical challenges faced by law enforcement and forensic teams during real investigations.

Few studies provide empirical case studies from forensic laboratories or actual legal proceedings, which makes it difficult to understand how chain of custody procedures are applied in practice. Moreover, there is a lack of standardized guidelines or performance metrics to evaluate different custody methods. Traditional human related issues, such as errors in documentation, inconsistent handling of evidence, and insufficient training of personnel, are often overlooked.

There is also very little research addressing integration challenges between modern digital tools and existing forensic frameworks. Privacy, scalability, and legal recognition of digital custody systems, particularly blockchain based solutions, remain underexplored in real world settings. Addressing these gaps could help develop a comprehensive framework that combines both technical solutions and human factors, ensuring effective, reliable, and legally admissible digital evidence management.

4. Chain of Custody (CoC)

CoC is a fundamental and critical process in the legal system, particularly in criminal and civil law cases. It refers to the chronological documentation and tracking of physical evidence from the moment it is collected at a crime scene or discovered through an investigation, through its handling, storage, and presentation in court. Typically, the chain of custody involves detailed records, including the names of individuals who had custody of the evidence, the dates and times of transfers, descriptions of the evidence, and any relevant information about its storage condition.[4] CoC is a pillar of DF (D4N6), which makes evidence gathered in a course of an investigation admissible in a court. It entails careful recording and monitoring of all the pieces of evidence since they are discovered up to the time when they are presented in court.[5] Chain of Custody (CoC) mainly works for collection of evidence which are used in investigations. It's a collection of evidences during investigation. It ensures evidence which is collected are the evidence are integrated, establish credibility, it supports legal admissibility and also preserves investigation incredibility. Chain of Custody is a systematic process of collecting, handling, documenting and preserving evidence that helps evidence is always intact and authentic. It also provides a record of who gathered the evidence, when the evidence was gathered, how it was treated, where it was kept at the time it was collected as evidence till the time it is presented in the court. CoC is important in the fields like criminal investigation, DF, legal processing where evidence needed only reliable and accurate.

The purpose of maintaining proper CoC to ensure that evidence is trustworthy, traceable, legally permissible. It helps investigators demonstrate that the evidence presented is original that cannot be altered, contaminated and substituted at any stage where evidence is gathered.

5. Workflow of CoC

Workflow defines how CoC works.

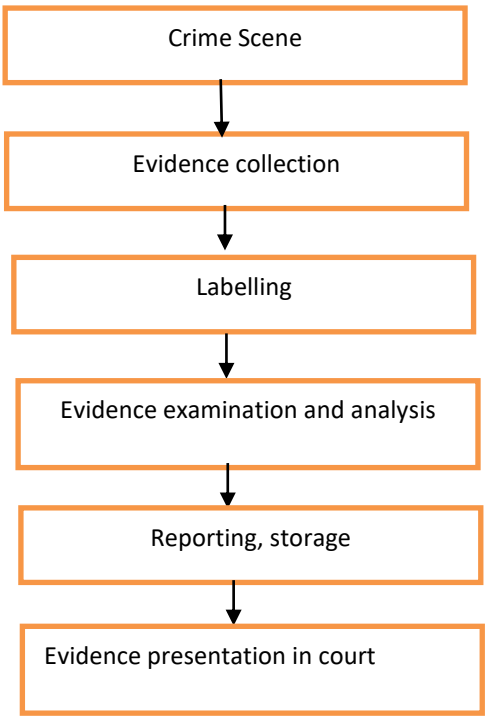


Figure 1: Workflow of CoC

5.1 Crime scene: It is starting point of investigation. Crime scene is secured that prevent unauthorized access and tainted. Investigators are carefully documents like digital evidence such as photos, videos, notes etc. It also helps to identify potential evidence. It maintains original condition of scene to identify original evidence and also maintaining is important because that cannot affect investigation.

5.2 Evidence collection: Evidence collection is second step of investigation where crime scene is originated evidence collection is first step how to collect evidence. All evidence is collected by forensics techniques that includes physical evidence such as fingerprints, blood samples, weapons or digital evidence such as mobile, laptops, photos, videos. Investigators use gloves, tools and containers to avoid damage. Each item is collected carefully and systematically.

5.3 Labelling: Labelling is third step where evidence is collected, after collection of each evidence carefully labelling is most important and evidence can be labelled properly. The label includes:

- Case ID and number
- Description of evidence
- Date and time collection
- Location where evidence found
- Name and signature of collector

Label step helps us to find that each piece of investigation is uniquely identified and traced throughout this process.

5.4 Evidence examination and analysis: Evidence examination and analysis is fourth step of investigation where we label evidence also the collected evidence is sent to forensics laboratory for detail examination of evidence. Experts will analyze the evidence using scientific methods such as fingerprint analysis, blood samples, DNA etc. All activities are included in documentations such as who collected the evidence, who handled evidence, what tests were performed. To make effective use of the evidence, the implementation of groups was introduced, which made it possible to bundle several pieces of evidence. The smart contract records the permissions of each group to each role. A user with a role which has access to a group, is able to upload an evidence hash to the smart contract. This will cause an event that will serve as the log of the chain of custody. An event contains information about the person who added the evidence, the group to which the evidence was added, and the evidence in the form of a SHA256 hash. This is all the evidence that was kept in the chain.[6]

5.5 Reporting and Storage: Reporting and storage is fifth step of investigation where after examine and after analysis the findings are documented in formal report. This formal report includes results, methods, tests and conclusions. The evidence is stored securely in controlled environments such as digital storage system also proper storage ensures the evidence is safe from loss, tampering and environmental damage.

5.6 Evidence presentation in Court: In final step, evidence is presented in court. The chain of custody is also presented to prove the evidence has been handled properly throughout the lifecycle. This will help to establish authenticity and reliability of the evidence.

6. Types of Evidence

We are mainly talk about five types of evidence. These evidence helps the investigators what type of evidence they collected.

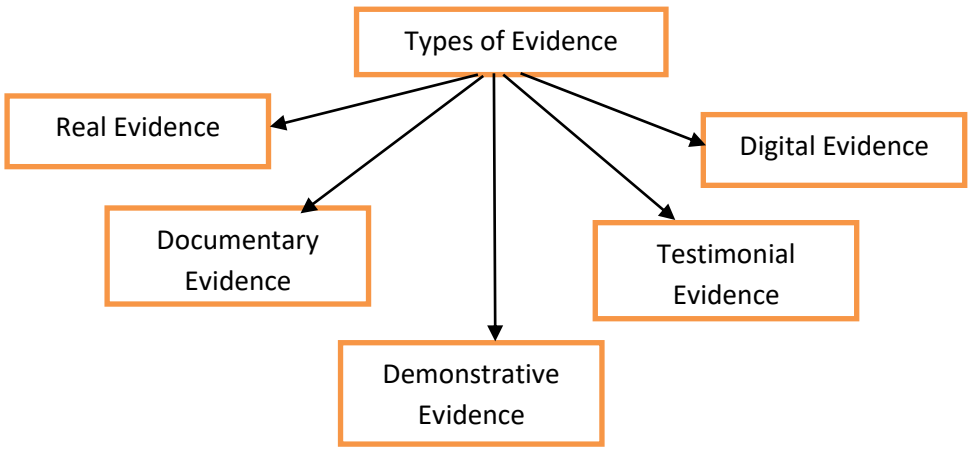


Figure 2: Types of Evidence

6.1 Real Evidence: Real evidence is the tangible object that is directly involved in crime. It can be seen, touched and examined physically. This type of evidence plays an important role because it provides a direct proof of what happened. Examples include weapons, fingerprints found at crime scene.

6.2 Documentary Evidence: Documentary evidence that include written or recorded evidence in documents. These documents help to understands the facts of any case. Examples include letters, emails, records that provide a permanent record that are verified and crosschecked for further use of documents in crime.

6.3 Demonstrative Evidence: Demonstrative evidence is used to explain facts in clear way so that court can understand complex information easily. It does not directly come from crime that it can represented something. Examples charts, maps, diagrams, models.

6.4 Testimonial Evidence: Testimonial Evidence is based on what a person says in court related to case whatever the investigation is. It is given by witnesses, victims or experts who share their knowledge related to case. Example include witnesses describes what they saw at crime scene.

6.5 Digital evidence: Digital evidence is that evidence which are stored and transmitted electronically. Digital evidence in the form of images, videos, CCTV footage etc. Example include data related to case such as CCTV footage, images and videos.

7. Why We Need Evidence

We need evidence because without it, our beliefs, decisions, and knowledge would be based only on assumptions, emotions, or guesses. Evidence acts like a foundation it supports what we claim to be true and helps others understand why they should trust or accept idea. In everyday life, evidence guides us in simple choices, like trusting a product because of reviews, or believing someone's story because they can show proof. Without evidence, it would be difficult to tell the difference between truth and falsehood. It also proves that the evidence presented in a case is the same evidence that was originally collected and that it is not been altered, tampered or contaminated along the way. The chain of custody is basically a documented timeline that shows who collected evidence, who handled it, where it was stored and how it was transferred from one person to another. Without this record, even strong evidence can be losing their value.

8. Importance of Evidence

Evidence is main aspect of investigation where investigators investigate about cases. CoC ensures that evidence remains trustworthy, accurate and legally acceptable throughout the process. Without proper handling of documentation evidence can lose their value in court. It also helps to maintain integrity. Evidence that collected always stores original condition without any alteration, contamination and damage. CoC provides a clear record of who has handled evidence, when it was handled and what actions were performed. This will help to prove the evidence is genuine and has not been tampered. If Chain of Custody (CoC) is incomplete, the evidence may be rejected. Another importance of preventing contamination and loss. Proper procedures for collecting evidence are collecting, storage and transfer ensures the evidence is protected from environment damage.

9. Concept of Hash Value in Evidence

A hash value is a unique digital fingerprint of a file or a piece of data. It is created using mathematical algorithm that converts any size of data into a fixed length of string of characters. Common hash algorithm includes MD5, SHA1 and SHA256. The cryptography libraries testing the MD5, SHA1, SHA224, SHA256, SHA384, SHA512 hashing algorithms on a set of data samples consisted of 34 files from different types of document and media (.docx,.pdf,.txt,.wav,.mp4,.JPG,.PNG) where the data size ranged between 12680 to 146943468 Byte.[7] When evidence is collected, its hash value is calculated. Every time the evidence is accessed or transferred; the hash is recalculated. If the hash value remains same, evidence is unchanged. If the hash value changes, evidence has been altered or tampered with.

Table 2: Hashing algorithm output structure

Sr. No.	Hashing Algorithm	Block size/Bit	Output Characters
1.	MD5	130	38
2.	SHA-1	168	45
3.	SHA-224	228	78
4.	SHA-256	289	34
5.	SHA-384	354	87
6.	SHA-512	516	456

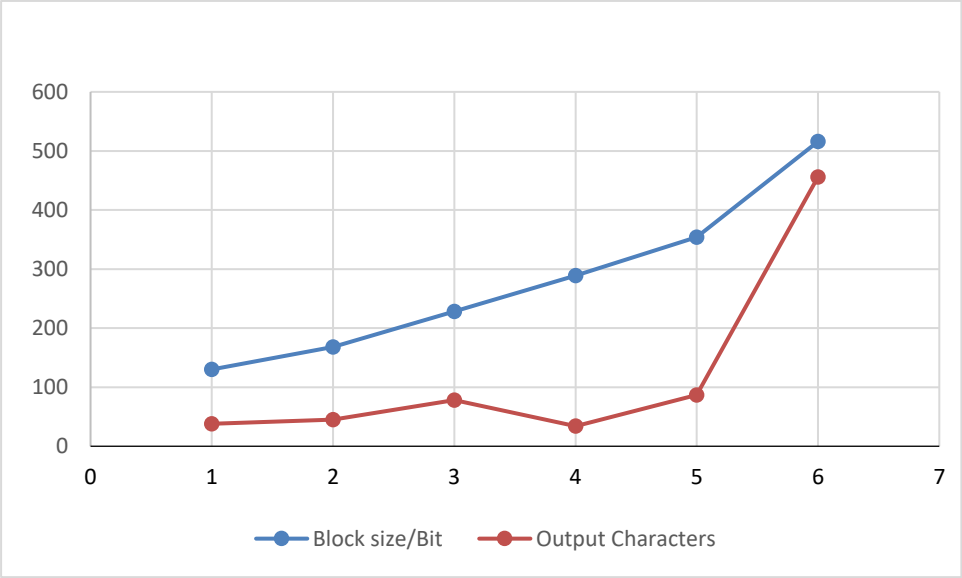


Figure 3: Block size and output characters of hashing algorithms

Blue line (Block size/ Bit) represents input data size. The orange line(Output characters) represents hash value that generates output. The behaviour of algorithm like SHA-256. Small or large file produces a fixed length hash value. Any small change in input completely have different output.

Example: How to convert the file into hash value so that no one can tampered it, altered it. I have a word file with named Practical 1. I want no one cannot be altered, tampered file. So I can produce hash value of file.

```
PS C:\> Import-Module NetTCPIP
PS C:\> Get-FileHash "Practical 1.docx"

Algorithm       Hash                                                                   Path
---------       ----                                                                   ----
SHA256          0CA462445A2C4A6CB1A9642531FFABD626EF5AACF8E68778EF0A657B994EF0DF       C:\Practical 1.docx


PS C:\>
```

10. Key Elements of Custody

The key elements of custody are:

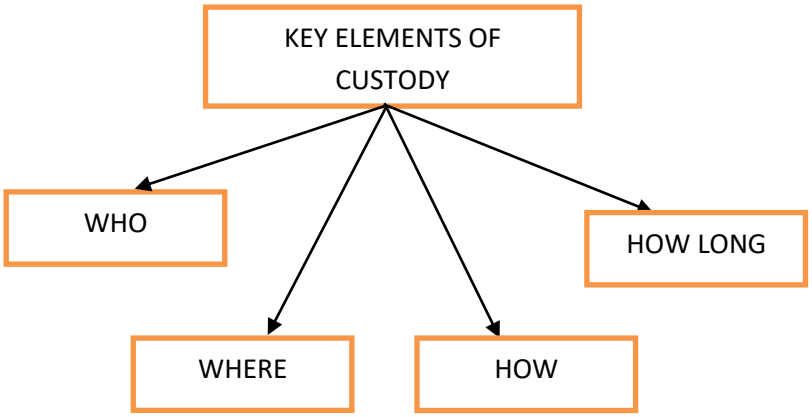


Figure 4: Key Elements of Custody

10.1 Who: The identity of individuals who had possession of the evidence at each stage. Names, roles, and signatures or digital confirmations of all handlers.[5] The person who has been collected evidence at crime scene. The collection of evidence in the form of digital and physical evidences. Example Photos, videos, phones etc.

10.2 Where: The location where evidence is collected. The exact location where the evidence was stored during each custody phase. Description of storage conditions, such as secure vaults, evidence lockers, or forensic labs.[5] The crime scene at what location what evidences are collected at what time evidences are collected, the location where crime scene occur.

10.3 How: The method of evidence transfer, including packaging, transportation, and security measures. Use of tamper-evident bags, seals, or secure digital transfers for data[5] The method of how to collect evidences how to transform it.

10.4 How long: The method of evidence transfer, including packaging, transportation, and security measures. Use of tamper-evident bags, seals, or secure digital transfers for data[5]

11. What are Digital Forensics (DF)?

The rapid development of the digital landscape has greatly widened the scope of DF, which has no longer been restricted to digital data stored in computers to be used as a part of the evidence in legal cases but now covers a wide range of activities and procedures. Ken Zatyko, the former

director of the Defense Computer Forensics Laboratory defined DF as "the application of computer science and investigative procedures for a legal purpose involving the analysis of digital evidence." It includes the analysis of legally applicable digital information that is stored or transferred in binary form, following such protocols as search authorization, a secure holding. CoC using validated tools, ensuring reproducibility, and providing comprehensive reports and potential expert testimony[8]. DF is a branch of Cybersecurity that focuses on identifying, collecting, analysing and preserving digital evidence from electronic devices that can be used in legal investigation. DF is the lifecycle of digital evidence, including its discovery to court testimony. It pulls information on a variety of sources such as online repositories, digital devices, and third-party storage systems. These data sources are essential for uncovering user activities and understanding events. Various models have been proposed to standardize the DF process, typically following a six phase progression: Identification, Collection, Preservation, Examination, Analysis, and Presentation[8]. DF (computer forensics) is the use of scientific methods for the identification, preservation, extraction and documentation of digital evidence derived from digital sources to enable successful prosecution. The objective of DF is to enhance and acquire legal evidence that is found in digital media. The current NIST definition of DF is the scientific procedures used to recognize and classify, collect, evaluate, and analyze the data while maintaining the level of integrity of the information throughout the forensics process. The purposes of DF are including forensic computing, forensic calculations and computer forensics[9].

12. Why Chain of Custody is Needed in DF

CoC is essential in DF to ensure evidence is authentic, untampered and legally investigate. Digital data is easily copied, altered, documented so DF is used to save the evidence safely.

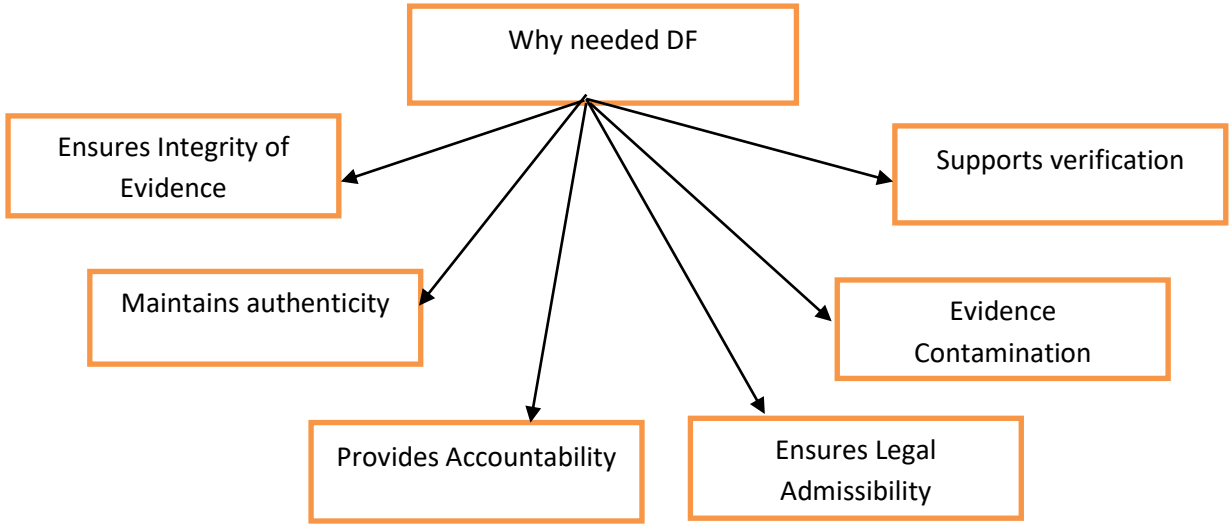


Figure 5: Why Chain of Custody is needed in DF

13. Importance of Chain of Custody (CoC)

13.1 Ensures Integrity of Evidence

Chain of Custody (CoC) ensures the integrity of digital evidence by maintaining a complete record of how the evidence was collected, transferred, stored, and analyzed. It helps demonstrate that the evidence has not been altered, corrupted, or tampered with during the investigation. Each step is properly documented so that the evidence remains in the same state as when it was originally collected.

13.2 Maintains Authenticity

Chain of Custody helps maintain the authenticity of digital evidence by proving that the evidence presented during an investigation or in court is the same evidence that was originally collected. It helps establish that the evidence is genuine and has not been replaced or manipulated.

Example: A hash value can be calculated when a file is collected and compared with the hash value calculated later. If both hash values are the same, it indicates that the file has not been changed.

13.3 Provides Accountability

CoC provides accountability by maintaining a record of every person who handles the evidence. Details such as who handled the evidence, when it was handled, where it was transferred, and why it was accessed are recorded. This creates transparency throughout the investigation and helps identify any unauthorized handling or access to the evidence.

13.4 Ensures Legal Admissibility

Proper Chain of Custody helps establish that digital evidence has been handled according to appropriate procedures. Courts may require investigators to demonstrate that evidence was properly collected, preserved, transferred, and analyzed. If there is a significant gap or unexplained break in the Chain of Custody, the reliability and admissibility of the evidence may be questioned.

13.5 Prevents and Detects Evidence Contamination

Digital evidence can be easily modified, deleted, or corrupted. Therefore, appropriate preservation methods are required to protect its integrity. Hash functions such as SHA-256 and SHA-512 can be used to generate a unique hash value for a file or digital evidence. If the evidence is modified, its hash value will normally change, helping investigators detect possible alteration or contamination.

13.6 Supports Verification Using Hash Values

Hash values provide an effective method for verifying the integrity of digital evidence. A hash algorithm converts digital data into a fixed-length value known as a hash value or digest. Investigators can calculate the hash value when evidence is initially acquired and calculate it again during later stages of the investigation. If the values match, it provides strong evidence that

the data has remained unchanged. Commonly used hash algorithms include MD5, SHA-1, SHA-224, SHA-256, SHA-384, and SHA-512. However, for modern forensic applications, stronger algorithms such as SHA-256 and SHA-512 are generally preferred over MD5 and SHA-1 because MD5 and SHA-1 have known collision vulnerabilities.

Practical example to convert file/evidences to hash value:

```
PS C:\> Import-Module NetTCPIP
PS C:\> Get-FileHash "Practical 1.docx"

Algorithm       Hash                                                                   Path
---------       ----                                                                   ----
SHA256          0CA4462445A2C4A6CB1A9642531FFABD626EF5AACF8E68778EF0A657B994EF0DF       C:\Practical 1.docx


PS C:\>
```

Conclusion

This study examined study of chain of custody in DF. The main issue we tried to solve in this work is how properly we can handle and protect evidence so that it remains trustworthy and acceptable in legal process. In today's worlds, crimes are often in electronic devices so that it become very important to ensure that evidence is collected from these devices is not altered, damage and tampered. To solve these problems, I focused on understanding the workflow of CoC, which explains how evidence is collected, documented, transferred and how it stored using hash function step by step. We also explain types of evidence and also explain why evidence is important, also explains the key elements and also try to understand why CoC is important in DF. This work aims to solve the problem of maintaining integrity, security authenticity and legal acceptance of the evidences.

Future Work

In future, this work can be expanded and improved by using advanced and automated tools to manage CoC. There are many automation tools to investigate evidences such as Digital Evidence Investigator (DEI), Cyber Triage. Automation can reduce human errors and make the process faster and accurate. There is also need to improve security methods such as hash function and encryption to protect evidence in better way. Future work also includes use of Artificial Intelligence (AI) to analyze digital evidences more efficiently and investigations in better way.

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ADVANCED FUNCTIONAL NANOMATERIALS: CHEMICAL DESIGN, CHARACTERIZATION AND REAL-WORLD APPLICATIONS

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Abstract
Recent advances in nanomaterials have resulted into their wide spread applications in healthcare, treatment of environmental pollution, energy conversion and storage, and industrial technologies. Increased utility of nanomaterials is due to their electronic, magnetic, optical and catalytic behaviour which is highly dependent on their size. A great range of synthetic methodologies have been developed to precisely control the shape, size and properties of nanomaterials. Health care sector has been given more emphasis with topics covering usage of functional nanomaterial in drug delivery, nucleic-acid vaccines, diagnostics, photothermal therapy, antimicrobial and enzyme-mimetic nanomaterials, and the barriers to clinical translation. The chapter concludes with a discussion of safety, scalability and sustainability, which determine whether laboratory advances become real-world products.

Keywords: Nanomaterials, Functional Materials, Colloidal Synthesis, Characterization, Nanomedicine, Lipid Nanoparticles, Water Treatment, Energy Storage, Industrial Nanotechnology.

1. Introduction

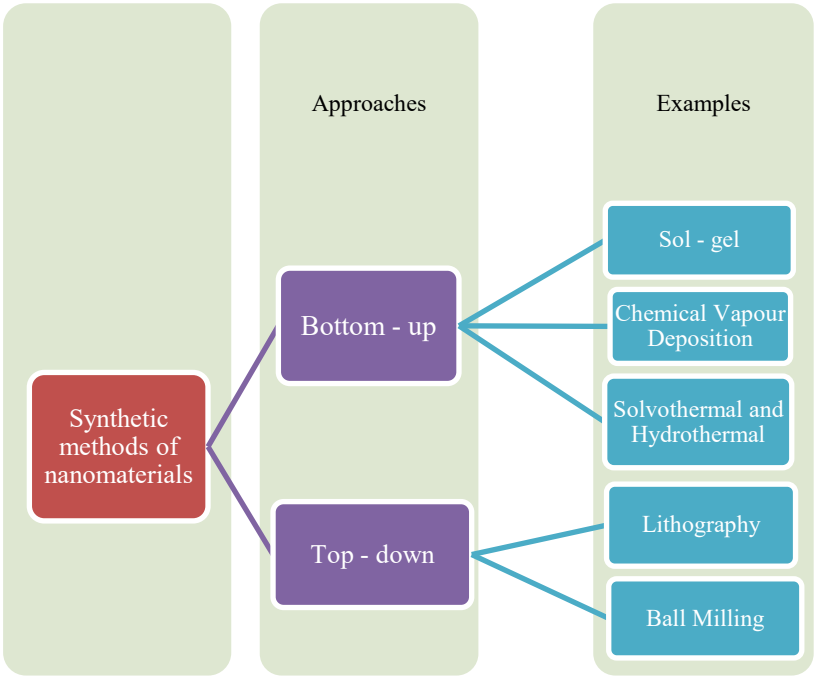
Nanomaterials/Nanoparticles are substance with size ranging from 1–100 nm range. At this scale, quantum confinement, Surface Plasmon Resonance (SPR), super-paramagnetism and a large fraction of under-coordinated surface atoms give rise to properties that differ markedly from those of the bulk. The practical consequence is that a chemist can tune a property such as emission wavelength, catalytic selectivity or magnetic response simply by controlling size, shape, composition and surface chemistry.

The field has matured to a stage where nanomedicines, nanostructured catalysts and nanoengineered electrodes are in clinical or commercial use. It can be clearly concluded from the literature that function follows structure. Anselmo and Mitragotri (2019) have listed the nanoparticle based drugs and drug delivery systems approved or in trials for clinical use, while Stark *et al.* (2015) have highlighted the brief history of materials such as carbon black, fumed silica and titanium dioxide along with emerging industrial applications of nanoparticles in

chemical industries. A successful application of a nanomaterial in real world application therefore demands rational chemical design, extensive characterisation and testing in actual operating conditions. The current chapter is organized for readers to provide this transition from design to application with particular emphasis to health care sector.

2. Chemical Design and Synthesis of Functional Nanomaterials

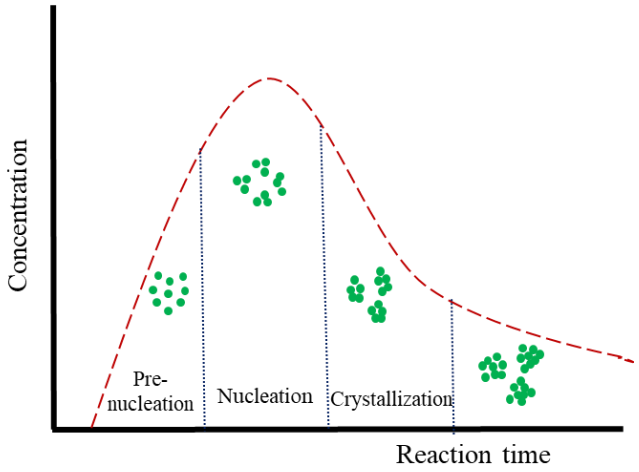
2.1 Design Principles: Top-Down and Bottom-Up Routes



Two basic synthetic strategies to synthetize functional nanomaterial include bottom – up and top – down approaches. In bottom – up strategies, an atom by atom is built to generate a nanomaterial in solution phase, while a macroscopic bulk material is reduced by methods such as ball milling, lithography, etc. in top – down approaches. Both approaches have their advantages and limitations. However, bottom – up strategies dominate the field because of the microscopic control and tunability and are generally compatible with scale up. Sol – gel process, Chemical Vapour Deposition (CVD), Hydrothermal and Solvothermal, Chemical Co-precipitation and templating methods convert atoms, ions or molecules into nanomaterials through nucleation and growth.

2.2 Mechanism of Growth of Nanomaterials

LaMer model developed by Victor LaMer explains the different phases during the formation of nanomaterials and how precise control over the size can be achieved on time scale. In Phase I, concentration of atoms/ions/molecules increases and they come very close to each but no particle is yet formed. Atoms or ions coagulate due to force of attraction leading to nucleation forming tiny nuclei. As the atoms or ions diffuse towards the nuclei, there is a gradual growth of particles in crystallization phase.



2.3 Colloidal and Wet-Chemical Synthesis

Synthesis of gold nanoparticles have gained immense attention and show how a controlled and well-designed synthesis can become a platform. Seminal work by Turkevich *et al.* (1951) on gold nanoparticle synthesis from the reduction of chloroauric acid using sodium citrate produces monodisperse, spherical gold nanoparticles. Even today it serves as a reliable method for generating seed particles for variety of functional nanomaterials such as plasmonic senors, biomedical devices, catalysts. Citrate layer capping on the nanoparticle surface can be easily replaced by different ligands like thiolate, polymers, DNA, etc. Gold nanoparticle chemistry is not restricted to spherical shape but they can be tailored to variety of shapes. Gold sol reduced with citric acid gave spherical and triangular nanoparticles while acetone, tannin, CO, oxalic acid, hydroxylamine gave irregular shapes. The size of particles varied with the concentration of citric acid. It concludes that reducing agent and experimental conditions have an important role in the shape of nanoparticles. Much of the efforts have been put in extending and controlling the shapes to non-spherical. Anisotropic nature associated with rods, prisms, shell shaped nanoparticles make them attractive for imaging. These non-spherical shapes can bring about bathochromic shift of the resonance wavelength.

The focus from gold nanoparticles has shifted to other metal, semi-conductor nanoparticles. Murray *et al.* (1993) reported the use of an organometallic reagent as the precursor for the synthesis of CdS, CdSe and CdTe nanocrystallites. Such materials have important application as semi-conductors. Spherical, uniform nanoparticles in the range of 1.2 to 11.5 nm were synthesized by injecting organometallic precursor into a hot coordinating tri-n-octylphosphine (TOP) solvent. The absorption spectra of the nanocrystallites showed the effect of quantum confinement. This method provided a simple, general and reliable path for production of near monodisperse nanoparticle which could be tuned across visible spectrum. Magnetic iron oxide particles, prepared by co-precipitation or thermal decomposition, are reviewed by Lu *et al.*

(2007), who show how they are subsequently protected and functionalised with silica, polymers or biomolecules for use in separations, imaging and therapy.

2.4 Sol–Gel, Templating and Surface Functionalization

Oxide and framework materials are prepared by sol–gel, hydrothermal and templating chemistry. Kresge *et al.* (1992) have compiled a review covering the design, synthesis, modification or tuning and application of magnetic nanoparticles. Their work demonstrated the use of surfactant liquid crystal as a template for the formation of hexagonal channels of mesoporous aluminosilicates. The tradition zeolites used in catalysis have been replaced by the mesoporous silica since the development of template mechanism. These materials have high surface area making them readily applicable in catalysis and drug delivery systems. Furukawa *et al.* (2013) demonstrated the metal-organic frameworks (MOFs) with strong bonds between organic and inorganic linkers. Such materials have been shown to have very high porosity with their inner surface easily tenable for functionalization. They have been used in gas separation, storage and catalysis. Two-dimensional materials such as graphene and MXenes, obtained by exfoliation or selective etching of layered precursors, add high conductivity and tunable surface terminations. Materials often in their native form have minimal practical application and hence chemical modification is required. Asahi *et al.* (2001) described a new nitrogen doped TiO2 based photocatalyst which is capable of doing visible light catalysis. They conceived that replacing oxygen in TiO2 anatase with an uncommon anion such as C, N, F, P or S would potentially yield a stable visible light activated photocatalyst. Calculation of density of a N doped TiO2 proved to be most effective in reducing band gap resulting from the mixing of P state of N with P states of oxygen. The active wavelength of the N doped TiO2 was found to be around 520 nm which makes it suitable for activation by fluorescent and incandescent light sources. Some of the features include reproducible photocatalytic activity, mass synthesis and environmentally benign nature of the material. It has been explored in the application of photooxidation of volatile organic materials, photocatalytic degradation of organic dye such as methylene blue and as an antibacterial agent. This work inspired the doping of metals with non-metals. Using solar light to break water into hydrogen is a longstanding challenge in material chemistry. It serves as a green option to future fuel in the view of crisis of non-renewable fuels. Wang *et al.* (2009) reported a semiconductor and a photocatalyst based on graphitic carbon nitride polymer. Such a polymer can be synthesized easily on a large scale and the raw materials are abundant. The uniqueness of this material lies in the fact that all known previous photocatalysts were inorganic, transition metal oxides or sulphides, while it is completely organic framework. The bandgap was calculated to be approximately 2.7 eV matching the blue region of the visible wavelength. Unlike organic compounds which have very low chemical stability in water, carbon nitride is very robust and exhibits thermal and chemical stability. Nanomaterials for medicinal use have been

designed using polymer coatings of polyethylene glycol (PEG) and other ligands which help in controlling circulation time, adsorption by protein and cellular uptake.

3. Characterization of Nanomaterials

The size, shape and surface have a crucial role in deciding the properties of nanomaterials and hence reliable techniques for characterization are equally important comparable to developing synthetic methodologies. A variety of characterization techniques are required for fully establishing the structure and properties of nanomaterials. Methods to study the morphology, crystal structure, crystallite size, composition, surface area, optical, magnetic properties in situ and in different operating conditions are needed. Table 1 lists some of the important techniques used in the characterization of advanced functional nanomaterials.

Table 1: Common characterization techniques for functional nanomaterials

Technique	Information Obtained	Typical Use / Limitation
TEM / HRTEM	Size, shape, lattice fringes, diffraction	Direct imaging; small sampling area, beam damage
SEM–EDX / AFM	Morphology, elemental mapping, topography	Films and bulk samples; limited resolution for tiny particles
XRD	Crystalline phase, crystallite size (Scherrer)	Peak broadening also reflects strain
N_2 physisorption (BET)	Specific surface area, pore-size distribution	Catalysts, adsorbents, electrodes
DLS / zeta potential	Hydrodynamic size, colloidal stability	Biased toward large particles
UV–Vis / photoluminescence	Band gap, plasmon resonance, aggregation	Fast, in situ monitoring
XPS / Raman / FTIR	Surface chemistry, oxidation state, defects, ligands	Surface-sensitive; careful interpretation needed

Direct images of nanomaterials for their shape and size is provided by electron microscopy. Scanning electron microscope (SEM) and transmission electron microscope (TEM) are the two variants commonly employed for nanomaterial imaging. Williams and Carter (2009) have explained how TEM can be useful in generating images covering morphology and lattice structure. Electron diffraction studies give chemical and structural information at atomic scale.

X-ray diffraction gives information about the lattice, crystallite structure based on the bulk sample. However, XRD requires powder samples while HRTEM can give precise information about lattice spacing in individual nanoparticle, identify crystallographic defects, count the number of graphene layers or measure the diameter of carbon nanotubes. Size of a crystalline material can be related to broadening of XRD peak by Scherrer equation. While the peak

broadening is assumed to be caused due to small size of nanoparticle, care must be taken to ensure as peak broadening can occur due to instrumental and lattice strain. Brunauer–Emmett–Teller analysis working on the principle of nitrogen adsorption remains the standard method for specific surface area measurement. It is particularly useful for catalysis, adsorbents and electrode design. Dynamic light scattering (DLS) provides the size distribution and hydrodynamic radius of nanomaterials suspended in solution. It is a complementary technique to electron microscopy. Optical spectroscopy refers to the interaction of electromagnetic radiation with the nanomaterial. UV-Vis-NIR spectroscopy is useful for studying localized surface plasmon resonance (LSPR) in metal nanomaterials. LSPR is an interesting phenomenon shown by metal nanoparticles, in which the collection of conduction electrons oscillates back and forth relative to the metal ion. When this frequency of oscillation matches with the wavelength of incident light, absorption of light takes place which is referred to as LSPR. It is exclusively exhibited by nanomaterials and the wavelength of absorption varies with the size and shape of nanomaterials. XPS is another characterisation technique to determine the elemental composition of a nanomaterial, to see if there are any contaminants at the surface of the nanomaterial and in what quantities they exist, to determine the chemical states of a nanomaterial. Nano oxides of Fe, Co, Ni tend to exhibit magnetic properties owing to their ferromagnetic behaviour. Magnetometry establishes the saturation magnetisation and superparamagnetic behaviour. It is useful to understand the strength of field required to separate and redisperse nanoparticles (Lu *et al.,* 2007). In biological and environmental settings, characterization must be repeated in the relevant medium, because protein coronas, ionic strength and dissolved organic matter can change the identity of a particle (Nel *et al.,* 2006). Increasingly, operando methods, in which a catalyst or electrode is examined while working, show that the structure of a freshly prepared sample can differ from that during operation.

4. Real-World Applications

4.1 Healthcare

Healthcare is the sector in which nanomaterial design is most demanding, because the material must be made under sterile, reproducible conditions, survive the biological environment, reach the intended tissue, perform its function and then be cleared safely. Pelaz *et al.* (2017) provide a broad overview, spanning therapeutics, diagnostics, imaging, regenerative medicine and antimicrobial strategies. Table 2 summarises the principal nanoplatforms and the roles discussed in the following subsections.

Table 2 outlines diverse nanoparticle platforms—lipid, albumin, gold, iron oxide, and silver—highlighting their distinct compositions, core biomedical applications like drug delivery, diagnostics, therapy, and antibacterial coatings, backed by seminal literature.

Table 2: Principal nanoplatforms in healthcare

Platform	Composition	Main Role	Source
Liposomes / albumin particles	Phospholipid vesicles; protein-bound drug	Reduced toxicity, improved solubility	Anselmo & Mitragotri (2019)
Lipid nanoparticles	Ionisable lipid, phospholipid, cholesterol, PEG-lipid	siRNA and mRNA delivery	Hou *et al.* (2021)
Gold nanoparticles	Au spheres, rods, shells	Colorimetric sensing, photothermal therapy	Elghanian *et al.* (1997); Hirsch *et al.* (2003)
Iron oxide nanoparticles	Magnetite / maghemite	MRI contrast, hyperthermia, nanozymes	Lu *et al.* (2007); Gao *et al.* (2007)
Silver nanoparticles	Ag, polymer-coated	Antibacterial coatings	Sondi & Salopek-Sondi (2004)

4.1.1 Nanocarriers for drug delivery

Nanocarriers improve the pharmacokinetics of drugs by prolonging circulation, solubilising hydrophobic agents, protecting labile cargo and altering biodistribution. Peer *et al.* (2007) distinguish passive from active targeting. Passive targeting relies on the enhanced permeability and retention (EPR) effect, first described by Matsumura and Maeda (1986), in which macromolecules accumulate in tumours because of leaky vasculature and poor lymphatic drainage. Active targeting adds ligands such as antibodies, peptides or aptamers that bind receptors overexpressed on cancer cells. Peer *et al.* (2007) further highlight stimulus-responsive and multifunctional designs in which a single particle carries drugs, imaging agents and targeting groups.

Several chemical design rules emerge from this literature. PEGylation reduces opsonisation and uptake by the mononuclear phagocyte system, extending circulation time; particle size must be large enough to avoid rapid renal clearance but small enough to extravasate in tumours; and surface charge influences both protein adsorption and cellular interaction (Peer *et al.,* 2007). Shi *et al.* (2017) add that newer carriers are engineered to release their payload in response to tumour-specific cues such as acidic pH or elevated enzyme levels, and are increasingly used to deliver combinations of chemotherapeutics, immunomodulators and nucleic acids. Anselmo and Mitragotri (2019) show that these principles have been realised in practice: PEGylated liposomal doxorubicin and albumin-bound paclitaxel are established examples of nanoparticle formulations that reached routine clinical use, mainly by reducing toxicity and improving formulation rather than by dramatically increasing tumour delivery.

This distinction is important because the early enthusiasm for EPR-driven targeting has been tempered by quantitative analysis. Wilhelm *et al.* (2016) analysed published data on nanoparticle delivery to solid tumours and found that a median of only 0.7% of the administered dose reached the tumour. Their analysis points to biological barriers, including sequestration in the liver and spleen, poor penetration of dense tumour stroma and variability between patients, as limiting factors. The finding has redirected the field toward understanding transport mechanisms, selecting patients whose tumours display strong EPR, and designing carriers that interact with the tumour microenvironment rather than relying on accumulation alone (Shi *et al.,* 2017).

4.1.2 Lipid Nanoparticles and Nucleic-Acid Therapeutics

The most visible clinical success of nanotechnology is the delivery of nucleic acids by lipid nanoparticles (LNPs). Hou *et al.* (2021) explain that LNPs are assembled from four components: an ionisable lipid, which is positively charged at low pH to complex the negatively charged nucleic acid and then becomes nearly neutral at physiological pH, a helper phospholipid, cholesterol, and a PEG-lipid that controls particle size and stability. After cellular uptake by endocytosis, protonation of the ionisable lipid in the acidifying endosome is thought to promote membrane disruption and release of the cargo into the cytosol. The authors note that the approval of an LNP formulation of small interfering RNA for hereditary transthyretin-mediated amyloidosis demonstrated clinical feasibility for the liver, where particles acquire apolipoprotein E and are taken up by hepatocytes.

Polack *et al.* (2020) reported that an LNP-formulated mRNA vaccine, BNT162b2, showed 95% efficacy against symptomatic Covid-19 in a large randomised trial. Beyond its immediate public-health impact, this result validated a modular platform: the nanoparticle chemistry remains largely constant while the encoded antigen can be changed rapidly. Hou *et al.* (2021) identify continuing challenges, including delivery to tissues beyond the liver, control of immunogenicity, storage stability and the need for ionisable lipids that are potent yet rapidly biodegradable. These issues are now the focus of research in gene editing, protein-replacement therapy and cancer vaccines.

4.1.3 Diagnostics and Biosensing

Inorganic nanoparticles are attractive diagnostic reagents because their optical or magnetic signals are strong and tunable. Elghanian *et al.* (1997) showed that gold nanoparticles carrying oligonucleotides aggregate when complementary target DNA is present, giving a visible red-to-purple colour change within minutes; the principle of target-induced aggregation underlies many colorimetric assays and lateral-flow tests. Gold, quantum dots and magnetic particles are also used as labels in immunoassays, as fluorescent probes for cell imaging and as contrast agents. Lu *et al.* (2007) describe how superparamagnetic iron oxide nanoparticles shorten the transverse relaxation time of water protons and therefore act as negative contrast agents in magnetic

resonance imaging, and how the same particles can be steered by magnetic fields or used for magnetic separation of cells and biomolecules.

A recurring requirement is that diagnostic particles retain their colloidal stability and signal in complex fluids such as blood, serum or saliva. Nel *et al.* (2006) explain that adsorbed proteins form a corona that alters size, charge and recognition by cells, so assays validated in buffer may behave differently in biological samples. Surface passivation with PEG or zwitterionic ligands and careful control of ligand density are therefore standard design steps.

4.1.4 Photothermal Therapy and Theranostics

Plasmonic nanoparticles convert absorbed light into heat. Hirsch *et al.* (2003) prepared silica core–gold shell nanoshells whose absorption was tuned to the near-infrared by adjusting the ratio of core diameter to shell thickness. Injected intravenously into mice bearing tumours and illuminated with a near-infrared laser under magnetic-resonance temperature monitoring, the particles produced localised heating that caused tissue damage in treated tumours, while controls without particles showed no comparable effect. The study is a clear example of how geometry, rather than composition alone, is used as a design parameter. Magnetic nanoparticles can similarly generate heat in alternating magnetic fields, a route known as magnetic hyperthermia that is also reviewed by Lu *et al.* (2007). Because the same particle can image, heat and carry a drug, such systems are often called theranostic, a theme that Pelaz *et al.* (2017) discuss as a major direction in nanomedicine.

4.1.5 Antimicrobial Nanomaterials and Nanozymes

Antimicrobial resistance has renewed interest in metal nanoparticles. Sondi and Salopek-Sondi (2004) showed that silver nanoparticles accumulate in the membrane of *Escherichia coli*, forming pits and increasing permeability, an effect that correlated with bacterial death. Silver is consequently incorporated into wound dressings and coatings of medical devices, although concerns about cytotoxicity and the emergence of resistance require control of dose and release.

A different concept is the nanozyme: Gao *et al.* (2007) found that magnetite nanoparticles, long regarded as inert magnetic carriers, possess intrinsic peroxidase-like activity, catalysing the oxidation of substrates by hydrogen peroxide. The activity depends on size and surface and can be used to amplify signals in immunoassays or to generate reactive oxygen species for antibacterial action, while retaining the magnetic recoverability of the particles. Nanozymes offer greater stability and lower cost than natural enzymes, although their selectivity remains inferior.

4.1.6 Safety and Barriers to Clinical Translation

The reactivity that makes nanomaterials effective can also cause harm. Nel *et al.* (2006) describe mechanisms of nanomaterial toxicity including oxidative stress, inflammation and release of toxic ions, and argue that physicochemical descriptors such as size, shape, surface charge and composition must be reported together with biological data. Long-term fate matters as much as

acute toxicity: biodegradable lipids, polymers and small iron oxide particles that enter normal metabolic pathways are easier to translate than persistent inorganic particles. Shi *et al.* (2017) and Pelaz *et al.* (2017) both note additional hurdles, namely batch-to-batch reproducibility, scale-up of multi-component formulations, regulatory classification of complex products, and the high cost of clinical trials. Successful translation has therefore tended to involve well-defined, relatively simple formulations addressing a clear clinical need, such as liposomes, albumin-bound drugs, iron oxide contrast agents and LNP-based vaccines (Anselmo & Mitragotri, 2019).

4.2 Environmental Remediation

Environmental applications exploit the high surface area, reactivity and recoverability of nanomaterials to remove pollutants and pathogens. Qu *et al.* (2013) review nanoadsorbents, nanostructured metals, nanomembranes, photocatalysts and antimicrobial agents for water and wastewater treatment, and conclude that cost, fouling, regeneration and the potential release of nanoparticles are the main barriers to full-scale use. Adsorption is a clear example of design for function. Yavuz *et al.* (2006) showed that magnetite nanocrystals of about 12 nm have markedly higher arsenic uptake than larger particles and can be recovered with a low-field magnet, combining high surface area with easy separation. Magnetic recovery, as reviewed by Lu *et al.* (2007), is a general strategy for preventing the release of nanoparticles into treated water.

Reductive remediation relies on nanoscale zero-valent iron (nZVI). Zhang (2003) summarised the preparation of iron particles of roughly 10–100 nm by borohydride reduction of iron salts and their use to transform chlorinated solvents, polychlorinated biphenyls and heavy-metal ions in water and soil. Coating the iron with a small amount of palladium creates a bimetallic catalyst that markedly accelerates dechlorination, and the particles can be injected as slurries into contaminated aquifers, which made nZVI one of the first large-scale environmental uses of nanotechnology. The same review notes, however, that bare particles aggregate and oxidise quickly, so surface stabilisers are needed to allow transport through porous media.

Heterogeneous photocatalysis uses light-generated electron–hole pairs to mineralise pollutants, but the wide band gap of TiO_2 restricts absorption to ultraviolet light. Doping strategies such as the nitrogen substitution reported by Asahi *et al.* (2001) extend absorption into the visible range, and carbon nitride offers a metal-free alternative (Wang *et al.,* 2009). Antimicrobial nanomaterials are applied to disinfection: the membrane damage caused by silver nanoparticles in *Escherichia coli* (Sondi & Salopek-Sondi, 2004) illustrates the mechanism, although Qu *et al.* (2013) caution that the release of silver ions must be controlled. In all cases practical deployment depends on immobilising the catalyst or adsorbent on supports or membranes and on demonstrating that treated water is free of residual nanoparticles and harmful by-products (Nel *et al.,* 2006).

4.3 Energy Conversion and Storage

Aricò *et al.* (2005) argue that nanostructuring benefits energy devices by shortening ion and electron diffusion paths, increasing electrode–electrolyte contact area and accommodating strain during cycling. Several landmark examples illustrate this. O'Regan and Grätzel (1991) built a solar cell from a mesoporous TiO_2 film, about 10 μm thick and with an internal surface area roughly a thousand times its geometric area, onto which a ruthenium dye was adsorbed. The cell converted about 7–8% of incident light to electricity, showing that a high-area nanocrystalline oxide could replace costly single-crystal semiconductors and launching research on dye-sensitised and, later, perovskite photovoltaics.

Electrocatalysis and fuel production follow a similar logic. Stamenkovic *et al.* (2007) found that the Pt_3Ni (111) surface has an oxygen-reduction activity about ten times that of Pt(111) and roughly ninety times that of the commercial Pt/C catalysts of the time, a result attributed to the altered electronic structure and reduced oxide coverage of the alloy surface; it has driven the development of platinum-alloy nanoparticles with lower platinum loading for fuel cells. For solar fuels, Wang *et al.* (2009) showed that carbon nitride can evolve hydrogen from water under visible light, although its quantum efficiency was modest and a sacrificial donor was required, which illustrates the gap between a proof of concept and a practical solar-to-hydrogen device.

In batteries, silicon is a striking case. Chan *et al.* (2008) grew silicon nanowires directly on stainless-steel current collectors and obtained lithium-battery anodes with a charge capacity close to the theoretical value for silicon, about 4200 mAh g^{-1} and roughly ten times that of graphite. The nanowire geometry accommodates the large volume change on alloying with lithium without pulverisation, and each wire maintains direct electrical contact with the substrate. A recurring design trade-off is evident here: nanostructuring raises surface area and shortens transport distances, but it also increases side reactions with electrolytes and can lower volumetric energy density. Aricò *et al.* (2005) therefore stress that nanomaterials should be selected according to the performance metric that matters for the device, whether power, energy, durability or cost, rather than by surface area alone.

4.4 Industrial Technologies

Industrial use of nanomaterials predates the term nanotechnology. Stark *et al.* (2015) show that tonnage-scale products include carbon black for tyre reinforcement, fumed and precipitated silica as fillers and rheology modifiers, titanium dioxide pigments, and nanoparticulate catalysts, and that flame-spray pyrolysis is a leading scalable route to such powders, in which a precursor solution is combusted to produce oxide particles with controlled size in a continuous process. Heterogeneous catalysis is a second major arena. Haruta *et al.* (1987) found that gold, long considered inert, becomes highly active when deposited as nanoparticles on oxides such as Co_3O_4, Fe_2O_3 and TiO_2: carbon monoxide was oxidised at temperatures well below 0 °C, far

lower than over conventional noble-metal catalysts. The result changed views of gold as a catalyst and led to applications in pollution control and selective oxidation.

Ordered porous solids provide well-defined catalyst supports. The uniform mesopores of M41S silicas (Kresge *et al.,* 1992) and the tunable cavities of MOFs (Furukawa *et al.,* 2013) allow active sites to be dispersed and substrates to be selected by size, which is exploited in fine-chemical synthesis and separations. In optoelectronics, colloidal cadmium-based quantum dots of the type reported by Murray *et al.* (1993) are used in displays because their emission colour is set by particle size, giving narrow, tunable emission. Table 3 consolidates representative examples from all four sectors.

Table 3: Representative nanomaterials and their roles in real-world applications.

Sector	Representative Nanomaterial	Key Function	Source
Healthcare	Lipid nanoparticles	mRNA delivery, endosomal escape	Hou *et al.* (2021); Polack *et al.* (2020)
Healthcare	Gold nanoshells	Near-infrared photothermal ablation	Hirsch *et al.* (2003)
Environment	Magnetite nanocrystals	Arsenic adsorption, magnetic recovery	Yavuz *et al.* (2006)
Environment	Pd-doped nanoscale iron	Reductive dechlorination	Zhang (2003)
Energy	Silicon nanowires	High-capacity Li-ion anodes	Chan *et al.* (2008)
Energy	Mesoporous TiO_2 films	Dye-sensitised solar cells	O'Regan & Grätzel (1991)
Industry	Supported gold nanoparticles	Low-temperature CO oxidation	Haruta *et al.* (1987)
Industry	Silica, TiO_2, carbon black	Fillers, pigments, coatings	Stark *et al.* (2015)

5. Conclusions and Outlook

Advanced functional nanomaterials emerge from a design cycle in which chemical synthesis sets composition and morphology, characterization verifies them, and application tests reveal what must be improved. In healthcare, this cycle has delivered liposomal and albumin-based drug carriers, mRNA vaccines and imaging agents, while photothermal agents, nanozymes and targeted systems continue to advance. In the environmental, energy and industrial sectors, magnetic adsorbents, nanostructured electrodes, catalysts and fillers show comparable maturity. Persistent challenges include limited delivery efficiency to target tissues, long-term stability under operating conditions, scalable and reproducible manufacturing, and the need to

demonstrate safety across the full life cycle. Progress will likely depend on combining in situ characterization with data-driven design, adopting greener syntheses, and engaging regulators and industry early, so that the next generation of nanomaterials is not only high-performing but also responsible.

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NANOPARTICLE: THE BEST VERSION OF CATALYST FOR THE SYNTHESIS OF THIAZOLE DERIVATIVES

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Abstract

Nanoparticle synthesis has gained significant attention in contemporary research due to its potential to enhance reaction rates and provide reusable, environmentally friendly, and time-efficient approaches to chemical synthesis. This study reviews various methods of nanoparticle synthesis, highlighting their respective advantages and limitations. Particular emphasis is placed on the application of nanoparticles as catalysts in the synthesis of thiazole derivatives and other heterocyclic compounds. The study aims to provide an overview of nanoparticle-based synthetic approaches and their potential to promote efficient and sustainable chemical transformations.

1. Introduction

Heterocyclic chemistry is class of organic compounds that has great advantage in various fields of chemistry related applications.(Abdel-Aziem 2026; Thorat *et al.* 2026) One of the best applications of such compounds is in pharmaceutical drugs and dedicated therapeutics related to rare diseases like cancer, tuberculosis, diabetics and so on. The heterocyclic compounds that contains heteroatoms like oxygen, nitrogen and sulphur. (Dawood *et al.* 2021; Makam *et al.* 2013). One of the heterocyclic compounds that is 2- amino thiazole which has attracted researchers because of its versatile applications in pharmaceutical as well as in the chemical field. This compound contains five membered rings with nitrogen and sulphur which make them important moiety for synthesis of various derivatives containing different substitutions. At C2-position of ring primary amine group is present which make more reaction and key intermediate in synthesis of different complex biologically active molecules.(Kumar and Singh 2021; Thorat *et al.* 2026) Over years of study as abroad spectrum drug it acts as anti-bacterial, anti-fungal, anti-microbial, anti-oxidant(Chugh *et al.* 2022), anti-HIV, anti-cancer(Serdaroğlu, Uludag, and Üstün 2026), anti-biofilm(Bhosale *et al.* 2024) and so on.

There are various methods for the synthesis of these biologically and industrially important chemical compounds. The methods include conventional method, ultrasonication method, grinding stone method(Edrees *et al.* 2018), microwave irradiation(Bhosale *et al.* 2023; Hadimani

et al. 2026; Narale *et al.* 2025), using various natural juices as catalyst, using different nano-particles, solvents like PEG-400(Adole *et al.* 2020), water, etc. These are some of the green methods which are less toxic, biocompatible, easy to handle and environment friendly. Use of nano-particles in the synthesis of thiazole ring containing derivative has attracted the researchers. This method is very easy, provides good yield, reusable and less time-consuming method. These nano-particles act as nano-catalyst in the synthesis of thiazole compounds. Generally, nano-particles contains metals like copper, zinc, cobalt, iron, manganese, Titanium and nickel. The important activity this nanoparticle is due to high surface area, stability and reusability.

1.1. What is the Nano-particles?

International Organisation for Standardization (ISO) as world organisation for national standards body defined the nano-particles as particles that has size between 1 to 100nm(Mota *et al.* 2025).

i. 1 to 100nm
ii. 100 to 500nm
iii. Larger than 500

The size and distribution of nanoparticles provide good surface area and selectivity while using it in reactions. On the basis of such small size and composite structure they are classified depending on their properties such as semiconductor, dielectric, metallic, magnetic and multi-functions which has their own applications in various fields. There are several methods for synthesis of nanoparticles.

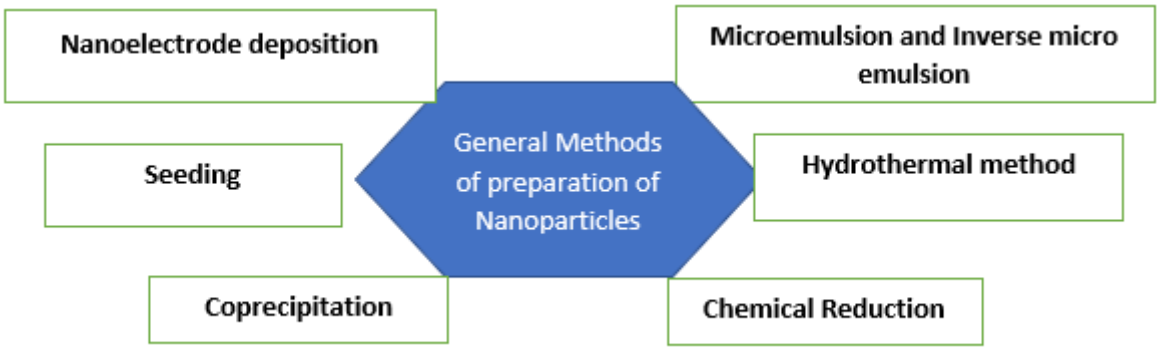


Figure 1: General methods of synthesis of nanoparticles (Szczyglewska, Feliczak-Guzik, and Nowak 2023)

The nanoparticles can be synthesised by conventional method and green methods. Depending on size, morphology, physical and chemical properties the nanoparticles are classified as organic, inorganic and carbon-based NPs. The morphology and the physical nature of nanoparticles make them effective in various applications. The surface and atomic arrangements in nanoparticles have greater importance in chemical synthesis and various industrial applications.

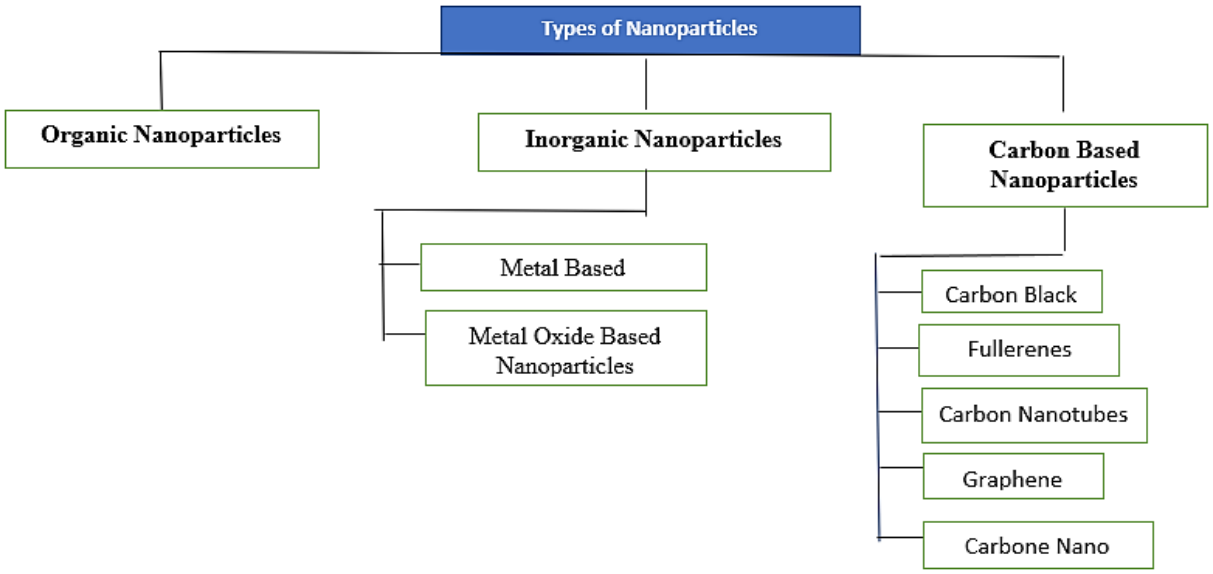


Figure 2: Different Types of Nanoparticles (Altammar 2023)

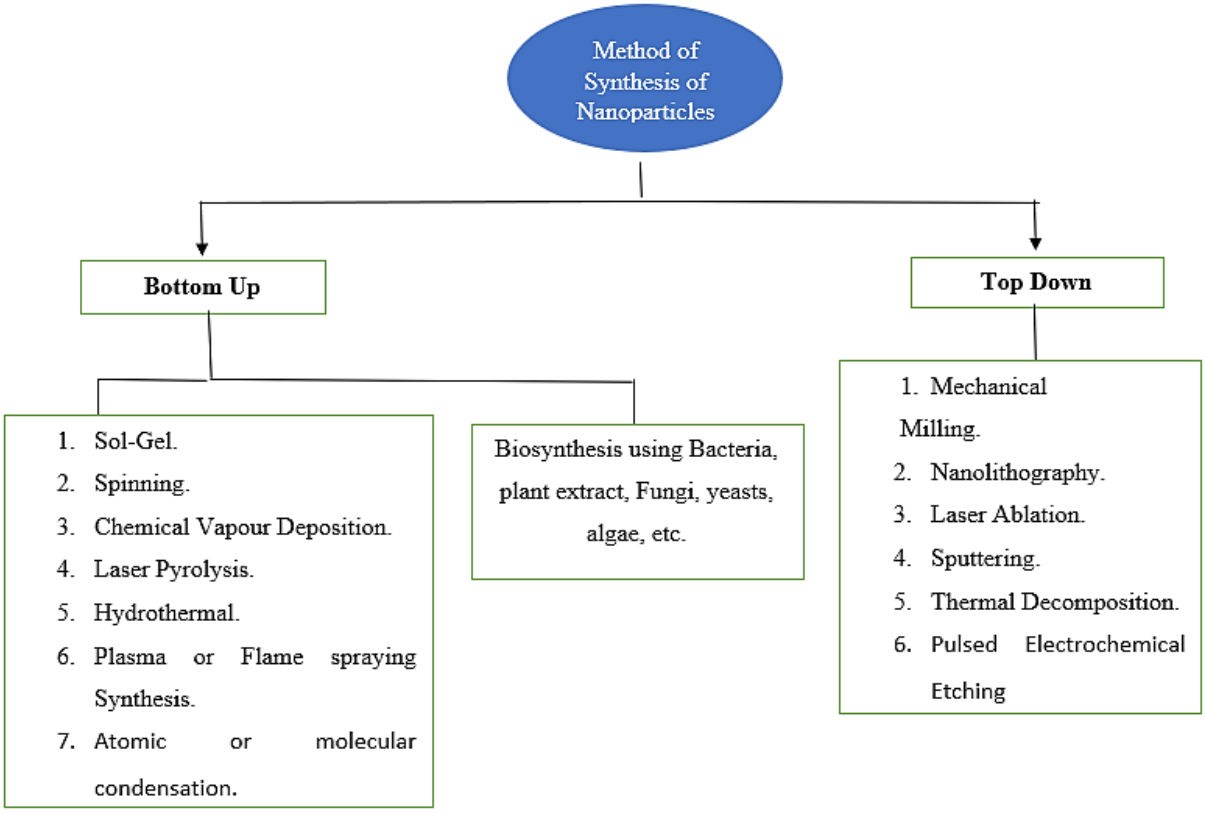


Figure 3: Different methods of synthesis of nanoparticles (Kumari and Sarkar 2021)

1.2 Types of Synthesis methods of Nanoparticles

A) Top-Down Approach: Here the macromolecules braked down in smaller particles and these particles arranged in building blocks by controlled reactions. The self-organisation of these particles take place which comes to get nanostructure. The disadvantage of this method is that the disturbance in physical and surface arrangements of atoms take place.

B) Bottom- Up Approach: In the bottom-up approach the nanoparticles get sized by cluster to cluster, atom to atom, molecule to molecule. The advantage of this method is that, less atomic imperfection and better physical and chemical properties.

1.3 Top- Down Approach

1.3.1 Mechanical milling

In this method a container is with milling balls which convert bulk materials into Nano-sized particles. The nanoparticles obtained by this method has advantage in energy storage, medicinal and energy transfer.

1.3.2 Nanolithography

Here the strong laser beam is used to produce nanoparticles and different nanoscale patterns can be produced on material surface. This technique is affordable and easy to use.

1.3.3 Laser Ablation

In Laser ablation strong beam of laser used to strike on metal surface which cause to generate nanoparticles. This method is very easy, cost effective and environment friendly which include generation of metallic, ceramic and carbon nanoparticle generation.

1.3.4 Sputtering

The highly strong energy beam strike to solid material surface and ejected particles get converted to nanoparticles. This method is better than the lithography but contains fewer contaminants.

1.3.5 Thermal Decomposition

Here nanoparticles get produced by heating the material at high flame. This method is not exactly a Top-Down method.

1.3.6 Pulsed Electrochemical Etching

The selective nanoparticles are produced in this method from the selective material.

1.4 Bottom Up approach

1.4.1 Sol-gel method

The involve formation of gel after condensation, hydrolysis then thermal decomposition of molecular precursors. Here particle size can be adjusted by changing the concentration of metal precursor.

1.4.2 Chemical Vapour Deposition (CVD)

In this method chemical precursor which can evaporate can be used as coating material over surface of substrate. This method is non-hazardous, long-shelf life, cost effective. CVD method provide strong, well sized and much active nanoparticles.

1.4.3 Lase Pyrolysis

Here a strong Laser beam is passed through gases mixture containing chemical precursor. Due to a strong heating, decomposition occur and convert these precursors into nanoparticles. This method provides cost effective and pure nanoparticles.

1.4.4 Hydrothermal

A very ambient to high temperature variations can be used for the formation of nanoparticles. The nanoparticles formed by this method has some good advantages that the physical and biological method.

1.4.5 Plasma or Fame spraying synthesis

Here both methods required high temperature but process are different. In plasma spraying method, plasma is used as ionised gas, which can vaporise precursor. Similarly, in Flame spraying method, a liquid precursor is vaporised and decomposed which results in the production of nanoparticles.

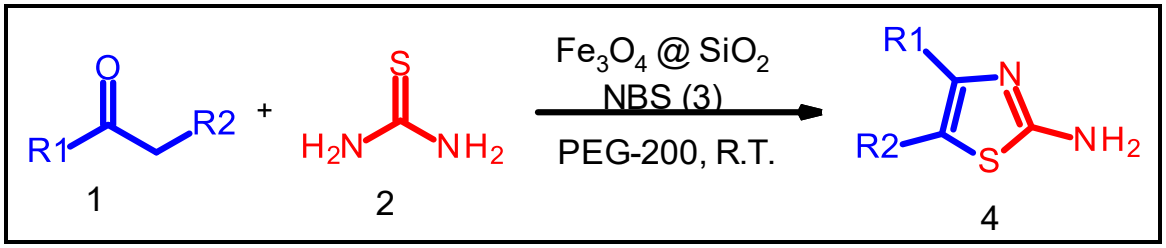
1.4.6 Atomic or molecular condensation

Formation of nanoparticles by this method has great attraction from researchers. Here inert gas can be used for attaining the temperature to vaporise the metal precursor. The liquid nitrogen can be used for cooling the gas.

1.5 Use of Nanoparticles for synthesis of 2-amino thiazole derivatives – green approach.

Heterocyclic compounds containing sulphur, Nitrogen and oxygen has great demand in pharmaceutical as well as in chemical industries. The world many research groups are working on such highly important and demanding compounds. 2-Amino Thiazole compounds which contain primary amine group attached to thiazole ring has shown number of biologically important activities such antibacterial, antifungal, anticancer, antituberculotic, antioxidant, etc. The purpose of synthesis of such important compound is to make human health better. These thiazole compounds can be synthesised by various methods like conventional heating and green methods like microwave irradiation, UV- irradiation, ball milling, using water as green solvent, PEG 300/PEG 400, Ionic liquids, different nanoparticles and Natural extracts. These all methods are non-toxic, easy to handle, hazard free, environment friendly. Now a day's synthesis of 2-amino thiazole compounds is synthesized using different nanoparticles. The use of this method is because it takes less time, cost effective and give good yield.

Javed Safari *et. al.* in 2015 used TiO_2 nanoparticles which was deposited over Fe_3O_4@ SiO_2 nanocomposites. The mixture of methyl carbonyl, Thiourea each 2mmol and N-bromosuccinamide(2.5mmol) with Fe_3O_4@ SiO_2 TiO_2 (10mmol%) in PEG-200 were reacted at room temperature. The progress of reaction was monitored by TLC the obtained crude washed with water, ammonified and recrystalised using absolute ethanol. Fe_3O_4 nanoparticles were synthesised by ultrasound and heating treatment. Fe_3O_4@ SiO_2 were synthesised by sol-gel method, similarly Fe_3O_4@ SiO_2 TiO_2 nanoparticles were also synthesised using sol-gel method Scheme No. (1). (Safari *et al.* 2015).



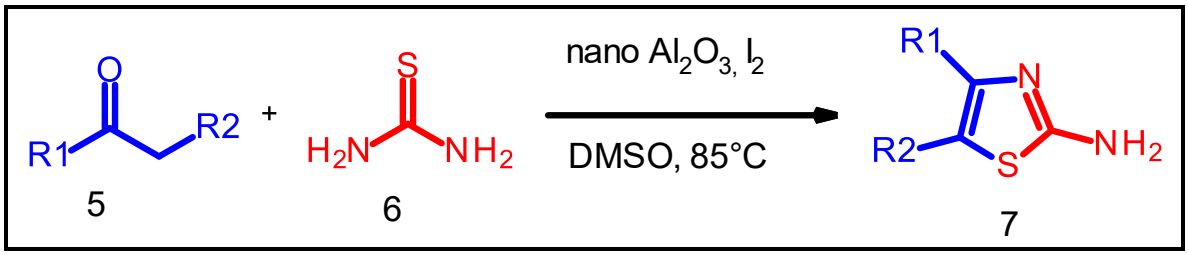
Scheme 1: General method for synthesis of 2-amino thiazole using Fe_3O_4@ SiO_2 TiO_2 nanoparticles as catalyst

Aluminium based nanoparticles were used as catalyst for synthesis of 2-amino thiazole by *Shokrani et. al.* in 2020. For the synthesis of these Aluminium based nanoparticles aluminium chloride, NH_3 and water by using heating method.

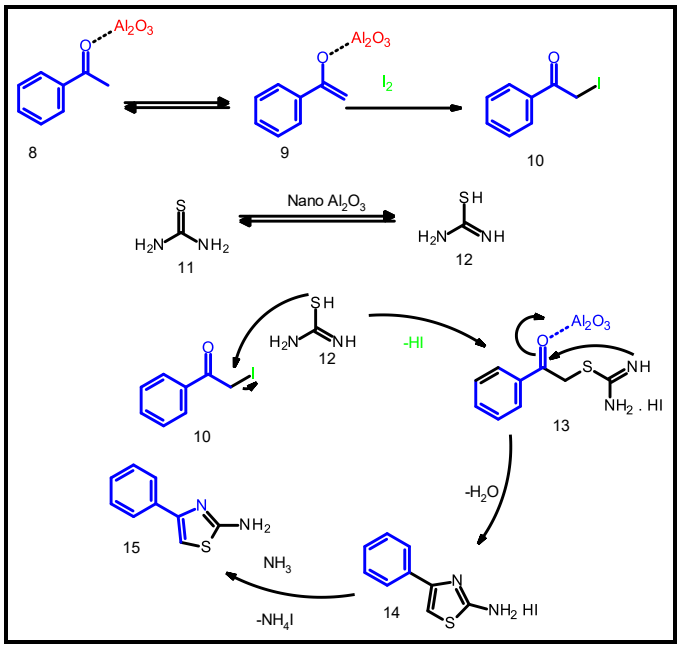
$$AlCl_3 + 3NH_4OH \rightarrow Al(OH)_3 + 3NH_4Cl$$

$$2Al(OH)_3 \rightarrow Al_2O_3 + 3H_2O$$

These synthesised nanoparticles were analysed by analytical techniques. 2-amino thiazole derivatives were synthesised by using nanoparticles of Al_2O_3. The mixture of methyl carbonyl(5mmol), thiourea (7.5mmol), I_2 (5mmol) and (1g) Al_2O_3 heated at 85˚C. The product obtained was much better that product obtained using general without catalyst **Scheme No. (2)**.(Shokrani, Zarnegar, and Safari 2020)

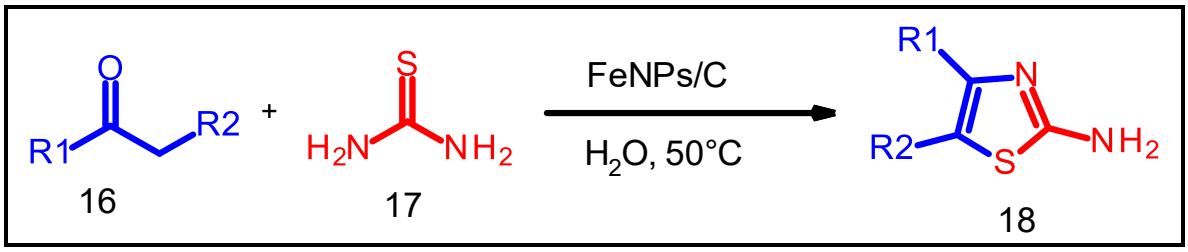


Scheme 2: Nano Al_2O_3 particle catalysed synthesis of 2- Amino thiazole derivatives



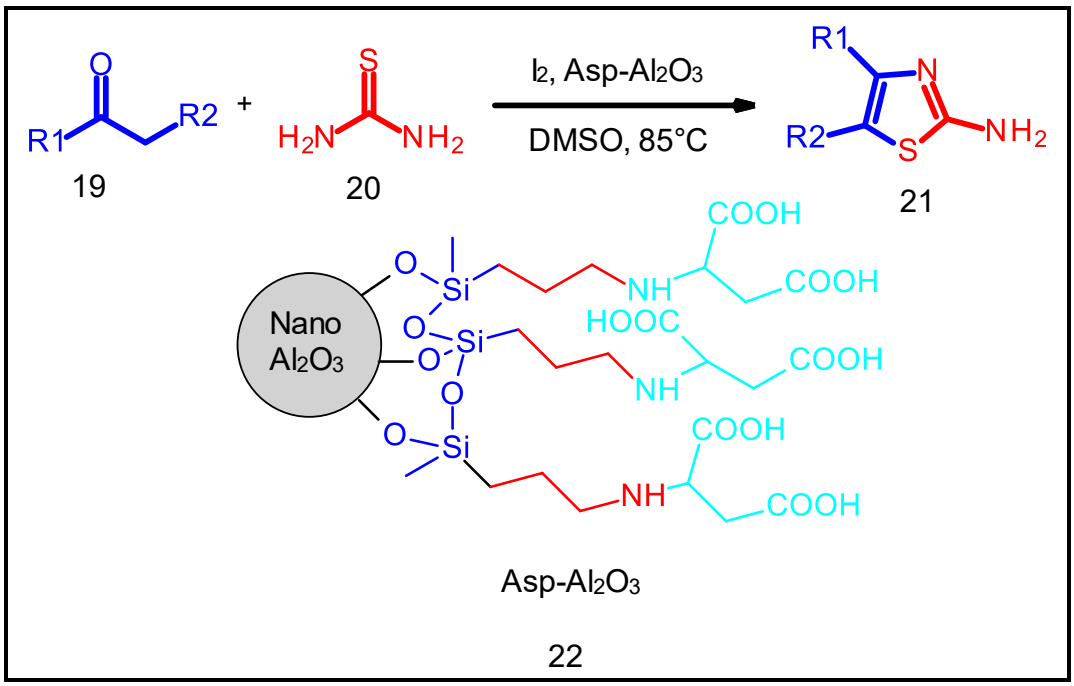
Scheme 3: Plausible mechanism for synthesis of 2-amino thiazole

Yang in (2025) developed a new method for synthesis of 2-animo thiazole derivatives using FeNPs in water as solvent. These FeNPs were synthesised using anhy. $AlCl_3$, suspension of Lithium, 4,4'-di-tert-butylbiphenyl (DTBB). Dur to large surface area, good accessibility and stability of these nanoparticles, they provide good yield of 2-amino thiazole. After number of trials by the author it was concluded that the quantity of nanoparticles FeNPs as (0.10), solvent-water, temperature of reaction 50˚C and time 60min provides good yield of 90-96% **Scheme No.(4)**.(Fan 2025)



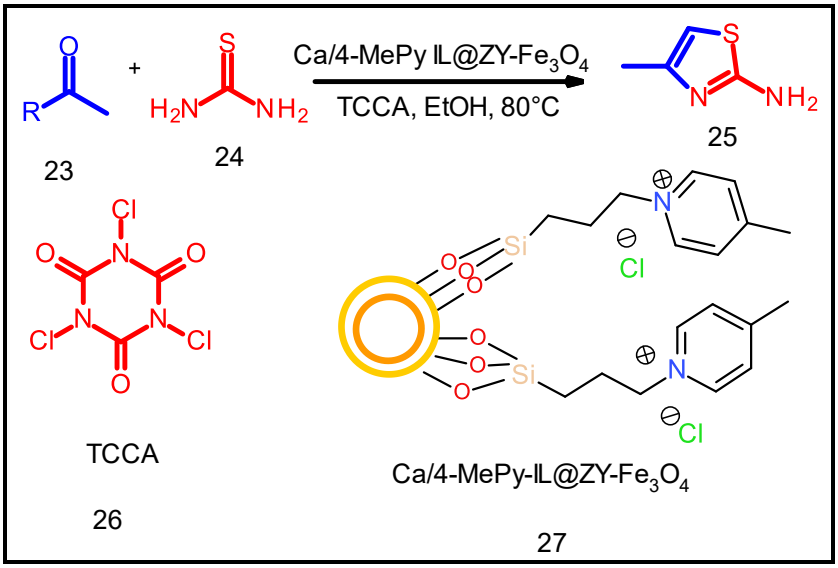
Scheme 4: FeNPs catalysed synthesis of 2-amino thiazole.

Z. Zarnegar et. al. in 2019 used Asparagine derived Al_2O_3 nanoparticles for the synthesis of 2-amino thiazole derivatives. This Asp- Al_2O_3 was synthesised first by precipitation method then modifications done with chloropropyltrimethoxysilane (CPTMS). The obtained precipitate heated with chloropropyl to get Asp- Al_2O_3 nanoparticles. Asp- Al_2O_3 nanoparticles act as good organo-catalyst for various reactions in organic synthesis. The as 2-amino thiazole derivatives were synthesised by one pot synthesis method in which Asp- Al_2O_3 nanoparticles as catalyst. The yield of the reaction obtained was 90-98% **Scheme No. (5)**.(Zarnegar, Shokrani, and Safari 2019)



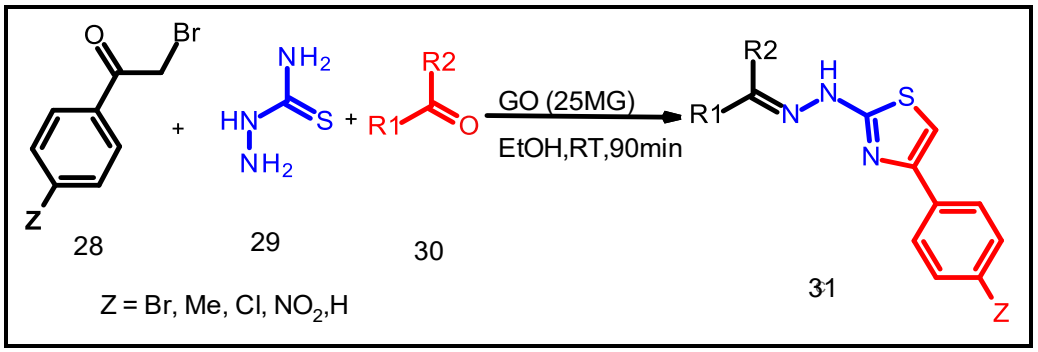
Scheme 5: Synthesis of 2-amino thiazole derivatives by using Asp- Al_2O_3 nanoparticles as catalyst.

Mehdi Kalhor et. al. used multifunctional ionic liquid nanocatalyst based on zeolite- Y, 4-methyl pyridinium chloride and calcium ions (Ca/4-MePy-IL@ZY -Fe_2O_3). For synthesis of 2-amino thiazole derivatives, 1.5mmol substituted acetophenone, 0.5mmol trichloroisocynuric acid (TCCA) and 0.01gm of Ca/4-MePy-IL@ZY-Fe_2O_3 was added in 3mL of ethanol. The above reaction mixture was heated for 25min at 80˚C. Completion of reaction was monitored using TLC and added 1mmol of thiourea. After completion of reaction nanoparticles were removed using external magnets and to this mixture 10% sodium bicarbonate solution were added. The precipitate obtained was washed with water. To neutralise the precipitate few drops of dilute acid added and then the obtained product was analysed by various analytical techniques **Scheme No.(6)**.(Kalhor, Vahedi, and Gharoubi 2023)



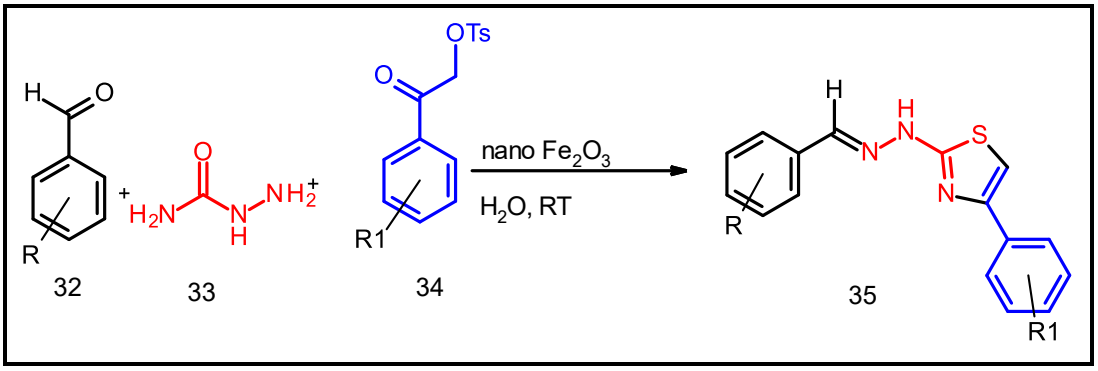
Scheme 6: Synthesis of 2-amino thiazole derivatives using Fe NPs as catalyst

In 2021, *Arindam Das et. al.* used graphene oxide nanoparticles as green catalyst for synthesis of thiazole derivatives. The yield obtained after the reaction was good as compare to general normal synthesis. The reason of choice of such nanocatalyst was, as it is metal free, less toxic, more surface area and good thermal stability. These nanoparticles were synthesised by heating the mixture of H_2SO_4, H_3PO_4, $KMnO_4$ and graphite powder. Here synthesis of thiazole derivatives was done by using this graphene oxide nanoparticles **Scheme No. (7)**.(Das *et al.* 2021)



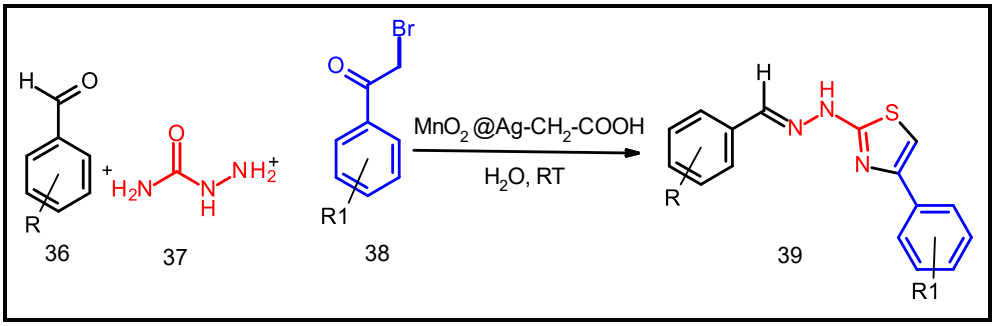
Scheme 7: Synthesis of thiazole derivatives by using Graphene oxide nanoparticles as catalyst

Rutikesh Gurav et. al. in 2021 did synthesis of thiazole ring containing heterocyclic compounds by using FeNPs derived from rust. The production of these nanoparticles was done by reported method. The reaction conditions were optimised from for synthesis of thiazole ring derived compounds by changing the different nanoparticles like CuO, ZnO, TiO_2, AgO_2 and Fe_2O_3. The yield of the reaction obtained was between (82-96) %. Hot filtration test was performed for understanding the heterogenous nature of FeNPs **Scheme No. (8)**.(Gurav *et al.* 2020).



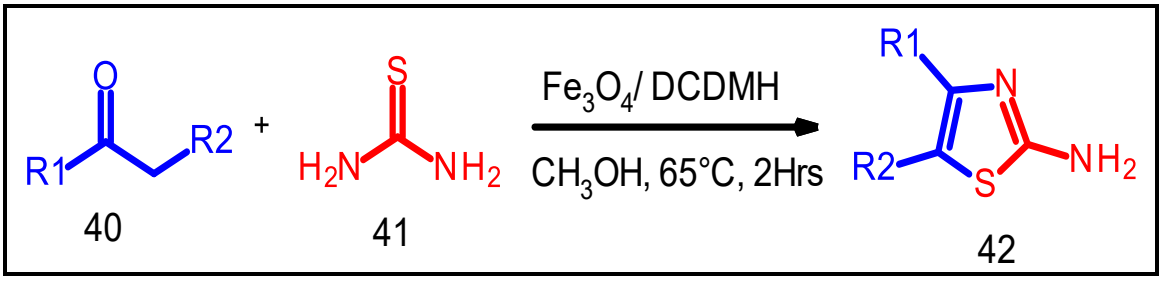
Scheme 8: FeNPs catalysed synthesis of thiazole derivatives

In 2025, *Phulewale et. al*. used MnO_2 @ Ag-s-CH_2-COOH as catalyst for synthesis of thiazole ring containing compounds. The *Psidium guajava* leaves extract were used for the synthesis of nanoparticles. The synthesised MnO_2 nanoparticles were coated with silver to enhance its reactivity. The mixture of equimolar quantity of substituted carbonyl compound, thiosemicarbazide and α-halo ketone were heated with addition of MnO_2 @ Ag-s-CH_2-COOH nanoparticles as catalyst and the reaction mixture were stirred at room temperature. The synthesised compounds were tested for various biological activities **Scheme No. (8)**.(Phulwale *et al.* 2025).

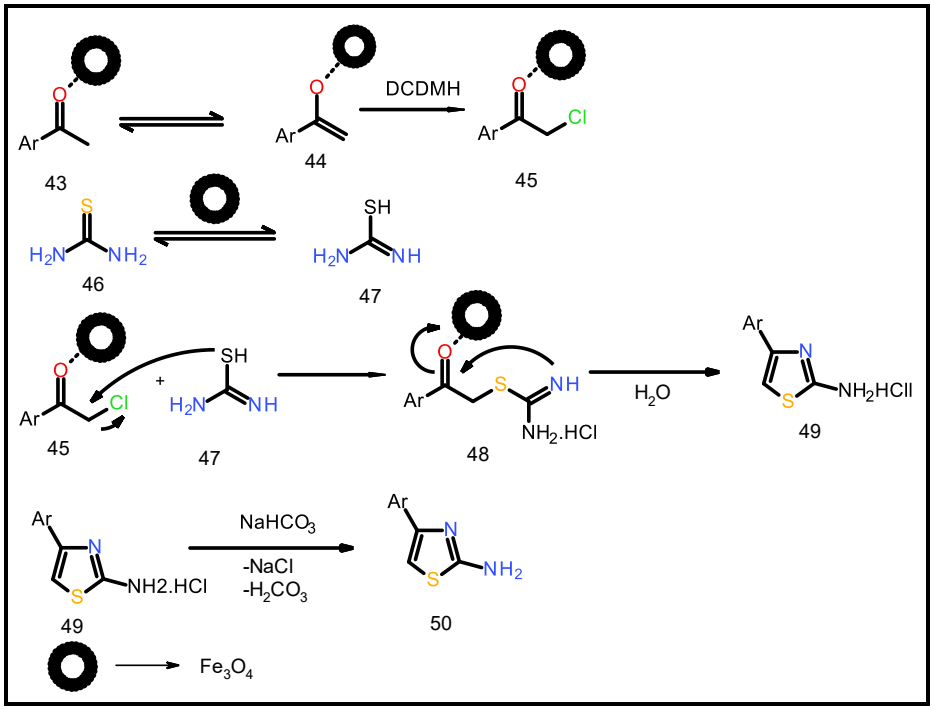


Scheme 8: MnO_2 catalysed synthesis of thiazole derived compounds

Masoud Sadeghi et. al. in 2016 synthesised the 2-amino thiazole using N-halo reagents 1,3-dichloro-5,5-dimethylhydantoin (DCDMH) as green, chlorinating reagent with Fe_3O_4 NPs as catalyst. The mixture of equimolar amount of methyl carbonyl, DCDMH and thiourea and Fe_3O_4 NPs in 2ml methanol heated at 65˚C temperature. The completion of reaction was monitored using TLC and the nanoparticles where removed using external magnet. The reaction is green, good yield of product, and easy separation using external field **Scheme No.(9)**.(Sadeghi, Safari, and Zarnegar 2016)

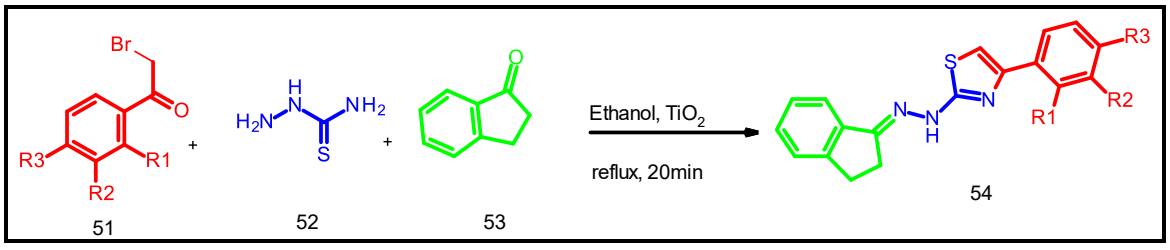


Scheme 9: Synthesis of 2-amino thiazole using Fe NPs



Plausible Reaction Mechanism for Synthesis of 2-amino thiazole using FeNPs

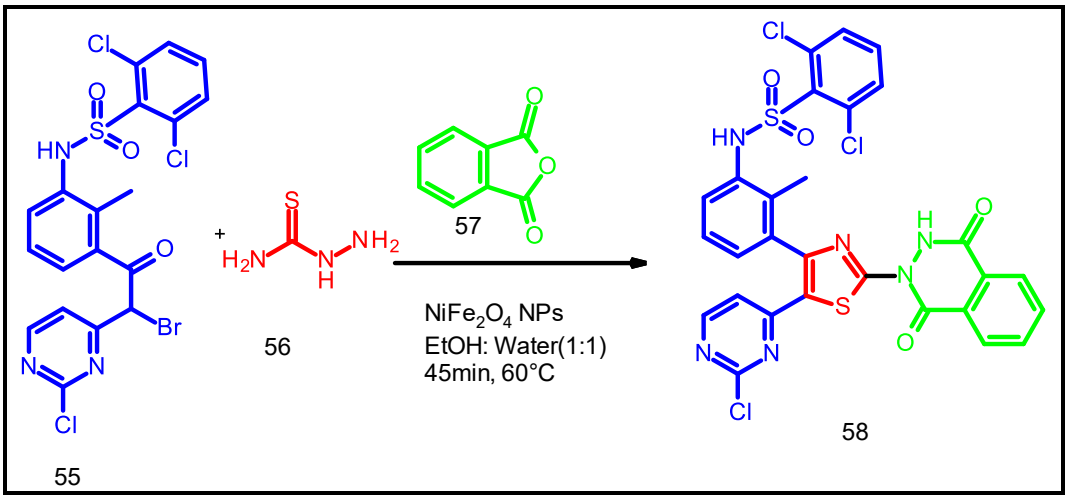
TiO_2 nanoparticles catalysed synthesis of thiazole derivatives was carried out by *Bankar et. al.* in 2026. During synthesis, due to presence of Lewis acidic sites od $Ti^{4+,}$ condensation and cyclisation occurs. The selection of TiO_2 nanoparticles is due to easily available less toxic and cheaper. Here the yield of the product was observed to high which make these nanoparticles more useful catalyst for the synthesis of thiazole ring containing compounds **Scheme 10)**.(Bankar *et al.* 2026)



Scheme 10: TiO_2 catalysed synthesis of thiazole amine derivatives

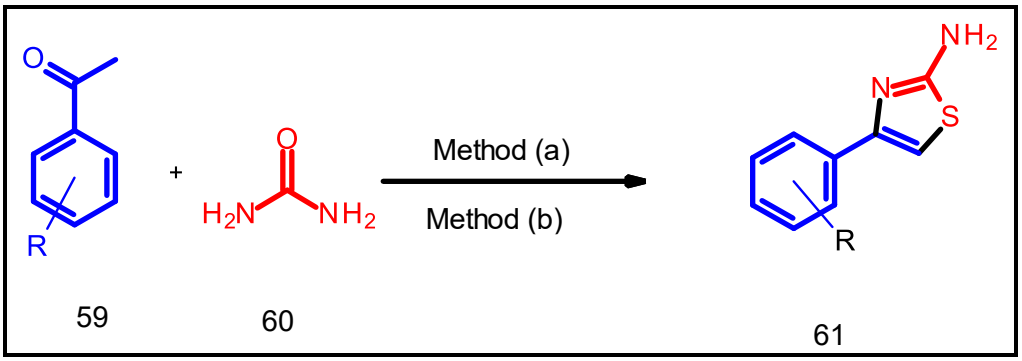
Satish Gundala and its co-workers in 2024 used $NiFe_2O_3$ nanoparticles for synthesis of thiazole amine derivatives. Sol-gel method was used for production of $NiFe_2O_3$ nanoparticles. Its structure and crystalline nature were confirmed by XRD data. The equimolar quantity of

substituted sulphonamides, thiosemicarbazide and substituted anhydrides were reacted in ethanol: water mixture with addition of $NiFe_2O_3$ nanoparticles as catalyst. The yield of the product obtained was 78-92%. After the completion of reaction, these nanoparticles were removed using external magnet **Scheme 11).**(Gudala *et al.* 2024)



Scheme 11: Synthesis of thiazole derivatives using of $NiFe_2O_3$ nanoparticles as catalyst

Ghorbani Vaghei et. al. in 2017 synthesised the 2-amino thiazole derivatives using a new catalyst discovered that is MNPs@SiO_2-PR-AP i.e. 4-amino pyridine silica. Fe_3O_4 was prepared by co-precipitation and MNPs@SiO_2 were production done by modified method of Stober. These synthesised nanoparticles were analytically evaluated by SEM, EDX, TGA-DTA and XRD. For synthesis of 2-amino 4-aryl thiazole, here two methods were employed. In method (a) the mixture of acetophenone, thiourea and N,N,N'N'-tetrabromobenzene-1,3-disulphonamide (TBBDA) or poly (N,N'-dibromo-n-ethyl-benzene-1,3-disulphonamide (PBBS) stirred and heated at 120-140˚C. In method (b)Thiourea, acetone, (TBBDA) was heated with the addition of MNPs@SiO_2-PR-AP in catalytic amount at temperature 80˚C. It was observed that MNPs@SiO_2-PR-AP with heating good yield as compared to method (b).(Ghorbani-Vaghei *et al.* 2018)



Method (a): TBBDA or PBBS, solvent-free, 120-140˚C.

Method (b): TBBDA/ MNPs@SiO_2-PR-AP, solvent-free, 80˚C.

Scheme 12: Synthesis of 2-amino thiazole amine derivatives MNPs@SiO_2-PR-AP as catalyst

Conclusion

Nanoparticles have emerged as promising materials in organic synthesis due to their potential to enhance reaction rates, improve catalytic efficiency, and support the development of reusable and environmentally friendly synthetic methods. This review highlights various approaches to nanoparticle synthesis, along with their advantages and limitations, with particular emphasis on their application as catalysts in the synthesis of thiazole derivatives and other heterocyclic compounds. The use of nanoparticles, in combination with green solvents and environmentally friendly reagents, offers opportunities to achieve good product yields, reduce reaction times, and minimize waste generation. Overall, nanoparticle-based catalytic approaches represent a promising strategy for promoting efficient, economical, and sustainable chemical transformations in organic synthesis.

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GREEN CHEMISTRY: PRINCIPLES, PROGRESS, AND PROMISE

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Abstract
Chemistry is viewed often as a science of creating pollution. Sustainable approaches to reduce waste, minimize the formation of hazardous substances, energy efficient synthesis, and promotion of renewable resources are together termed as Green Chemistry. This chapter explores the concept of green chemistry covering the historical background, fundamental principles, highlights the important advances in the field with emphasis to green solvents, catalysts, renewable starting materials and circular economy practices. The chapter also covers the various assessment tools such as E-factor, atom economy and life cycle assessment. Despite significant progress, challenges such as technological limitations, high implementation costs, and inadequate regulatory support continue to hinder widespread adoption. Emerging technologies, including artificial intelligence, electrocatalysis, synthetic biology, and flow chemistry, offer promising opportunities to advance sustainable chemical manufacturing and reduce the environmental impact of the chemical industry.

Keywords: Green Chemistry, Twelve Principles, Sustainable Chemistry, Waste Prevention, Catalysis, Renewable Feedstocks, Green Solvents, Circular Economy, Life Cycle Assessment, Sustainable Chemical Manufacturing.

1. Introduction

Green chemistry is one of the few concepts that has revolutionized the entire face of modern chemistry in a fundamental way. The development of this concept took place in the early 1990s when Paul Anastas and John Warner developed the field through their collaborative work at the United States Environmental Protection Agency (EPA). This concept has since been formalized through their pioneering text 'Green Chemistry: Theory and Practice' in 1998, where they enunciated twelve principles that would be used to redirect the science of chemistry from waste and hazard to efficiency and sustainability (Anastas & Warner, 1998). Ever since that foundation, green chemistry has transformed from a largely visionary concept into a robust scientific system adopted by researchers, industrial chemists, regulatory bodies, and policymakers worldwide.

The need for such a framework was not just theoretical. By the twentieth century it had become very clear, that the chemical industry, essential as it was to modern life, had significant environmental and public health costs. Industrial processes released millions of tonnes of toxic

by-products annually, consumed non-renewable resources at an enormous rate, and generated hazardous waste that was extremely difficult and cost inefficient to remediate. The U.S. Toxic Release Inventory, first published in 1988, brought these costs into public view, revealing that American manufacturers alone discharged billions of pounds of toxic chemicals into air, water, and soil each year (EPA, 2021). Conventional approaches to managing chemical risk focused largely on end-of-pipe controls, scrubbers, containment systems, and waste-treatment facilities. Green chemistry proposed something more radical: designing hazard out of chemical processes before it ever arose, i.e, to stop the problem before it even conceptualizes.

This chapter examines chemistry in depth. It traces the origins of green chemistry and unpacks each of the Twelve Principles of green chemistry, defines the major methodological advances that have followed green chemistry, and evaluates progress against the enormous challenges that remain for green chemistry.

2. Historical and Intellectual Background

However, one is unable to talk about the development of the principles of green chemistry without considering the general context of the environmental movement that preceded it. Silent Spring by Rachel Carson, published in 1962, warned the general public of the risks related to the use of organochlorine pesticides, which triggered the development of the modern environmental regulatory system; the Clean Air Act (1970), Clean Water Act (1972), and the establishment of the EPA took place in the next ten years (Colborn *et al.,* 1996). These regulations led to noticeable progress in the improvement of air and water quality; however, their effect was limited to regulation of chemical discharge, and not to challenging of the production of hazardous substances at all.

In the 1990s, a new generation of chemists trained in this environment started asking this difficult question. Anastas was one of the key contributors who formulated the ideas of pollution prevention at the molecular level: it is possible to say that waste is not an inevitable result of synthesis but a sign of inefficient design (Anastas & Williamson, 1996). It should be noted that the ideas of pollution prevention have roots in other intellectual trends. For instance, Barry Trost introduced the idea of atom economy in 1991; it provided the quantitative evaluation of the efficiency of a synthesis through the calculation of what percentage of reactants is included in the target product.

These principles offered chemistry a theoretical platform for describing its work and provided metrics to measure progress in terms of quantifiable figures. The birth of this movement happened with the introduction of the Twelve Principles of chemistry by Anastas and Warner. Soon after, support for this discipline was gained in an increased manner. The Green Chemistry Institute came up in 1997 and was incorporated into the American Chemical Society later on. At the same time, the Presidential Green Chemistry Challenge Awards, which were started in 1996, awarded those firms that proved green techniques to be profitable.

3. The Twelve Principles of Green Chemistry

The twelve principles articulated by Anastas and Warner remain the intellectual backbone of the field. They are worth examining not merely as a checklist but as an integrated philosophy of chemical design (Anastas & Warner, 1998).

3.1 Prevention

The first and maybe the most fundamental principle states that it is better to prevent waste formation than to have to treat or mitigate it after creation. Even though the statement seems self-explanatory, it implies some important consequences: chemists need to consider the full material balance of the reaction not just taking the product into account but also all solvents, reagents and by-products used. The E-factor introduced by Sheldon exemplifies the said principle. In pharmaceutical syntheses E-factors typically vary between 25 and 100, which means that in such processes 25 to 100 kilograms of waste are formed per one kilogram of active pharmaceutical ingredient; in fine chemicals production the E-factors are usually in the range from 5 to 50 (Sheldon, 2007). Bringing down the numbers is the main challenge facing green pharmaceutical chemistry.

3.2 Atom Economy

The atom economy index defined by Trost calculates what share of the molecular weights of the reagents is included in the molecule of the product: atom economy (%) = (molecular weight of desired product) / (sum of molecular weights of all reagents) × 100 (Trost, 1991). The theoretical maximum of 100% atom economy is achieved during addition reactions when all atoms of all reagents are used in the formation of the product. Substitution reactions producing stoichiometric amount of salt by-products can have much lower atom economies of up to 50%. The problem with the index is that it does not take into account the solvents, catalysts and energy consumed, which gave rise to other indices, including reaction mass efficiency (Curzons *et al.,* 2001).

3.3 Less Hazardous Chemical Syntheses

It is desirable to design synthetic methods that use and produce chemicals that have little or no toxicity to human beings and the environment. This tenet entails integrating the toxicological factors into the synthetic design of chemical reactions. The "benign by design" concept has been thoroughly elaborated by DeVito (1996) who has claimed that due to the knowledge of the structure activity relationships the chemists are able to alter the molecular structure in order to preserve desired properties and reduce the hazard by, for example, replacing persistent organohalogens with easily degradable groups.

3.4 Designing Safer Chemicals

Closely related but distinct from the previous principle, this guideline directs chemists to design chemical products that are fully effective while minimising toxicity. The distinction matters: principle three concerns the synthesis route; principle four concerns the product itself. Work in this area has been particularly active in agrochemistry, where older broad-spectrum

organophosphate and organochlorine pesticides have gradually been replaced by more selective compounds with lower mammalian toxicity and shorter environmental persistence (Lamberth *et al.,* 2013).

3.5 Safer Solvents and Auxiliaries

Solvents are the biggest part of mass in most pharmaceutical and fine chemical reactions, typically comprising about 80-90% of process mass. Much of the traditional solvents including halogenated hydrocarbons like dichloromethane and chloroform, as well as polar aprotic solvents like dimethylformamide and N-methylpyrrolidone are considered toxic, carcinogenic and persistent in environment (Constable *et al.,* 2007). Therefore the research of greener alternatives has involved supercritical fluids, ionic liquids, deep eutectic solvents, bio-based solvents. Industrial companies like AstraZeneca, GlaxoSmithKline and Pfizer have developed solvents guides that assess solvents based on several hazard, environmental, and health factors (Henderson *et al.,* 2011).

3.6 Design for Energy Efficiency

Energy consumption of a chemical process has both environmental and economic implications and must be reduced as much as possible. Wherever possible chemical synthesis reactions should be performed under ambient conditions of temperature and pressure. According to Jiménez-González *et al.* (2011) the pharmaceutical industry is roughly 50 times more energy demanding per unit of production than the automotive industry. Therefore a lot of efforts have been done on development of ambient temperature catalysis, microwave-assisted reactions, and continuous flow processes which are energy efficient as compared to conventional batch processes (Glasnov & Kappe, 2007).

3.7 Use of Renewable Feedstocks

Raw materials (feedstocks) should be renewable rather than depleting where possible. Petrochemical industry traditionally used fossil fuel resources like crude oil, natural gas, and coal as energy sources and feedstocks. One possible alternative is biomass from which sugar, fatty acids, terpenes, and lignin could be obtained and used as initial materials for manufacture of various chemicals. According to Bozell and Petersen (2010), who reviewed the top value added chemicals available through biomass according to U.S. Department of Energy, various organic compounds, including succinic acid, levulinic acid, and furans, could be synthesized via fermentation or catalytic transformation of lignocellulosic biomass.

3.8 Reduce Derivatives

Derivatization, the use of blocking groups, protection-deprotection strategy, and transient modification of physical and chemical process need to be minimized or avoided, if possible, because all these techniques require the use of extra reagents and produce waste. In their work, Wender *et al.* (2008) have presented a new concept called “step economy,” which is a

continuation of the idea of atom economy and claims that an optimal synthetic route involves converting the reactants to product in the minimal number of steps with maximum structural complexity achieved in each step. Multicomponent reactions in which three or more reactants combine in a single step to form structurally complex product are examples of such routes.

3.9 Catalysis

Catalytic reagents should be used whenever possible and especially when they are highly selective. This principle goes hand in hand with several others because using catalysts improves the atom economy, reduces waste, and allows carrying out the reactions under milder conditions. Asymmetric catalysis which allows producing one enantiomer from the pair of stereoisomers was awarded the 2001 Nobel prize in Chemistry to William Knowles, Ryoji Noyori, and K. Barry Sharpless. Asymmetric catalysis has dramatically changed the way drugs are manufactured (Noyori, 2002). Modern advances in this field include organocatalysis, photoredox catalysis, and enzymatic catalysis, all of which provide different benefits in terms of selectivity, functional group compatibility, and mild conditions (MacMillan, 2008).

3.10 Design for Degradation

Design for Degradation means designing chemical products in such a way that after they have performed their functional task they degrade into non-toxic products and do not accumulate in the environment. This principle directly applies to persistent organic pollutants and includes compounds like polychlorinated biphenyls (PCBs), per- and polyfluoroalkyl substances (PFAS), and some flame retardants. These pollutants resist biodegradation and accumulate in the environment through the food chain (Gavrilescu *et al.,* 2015). Designing degradable compounds requires knowledge of metabolic and photochemical pathways of degradation of organic compounds and designing appropriate functional groups to promote degradation.

3.11 Real-Time Analysis for Pollution Prevention

The analysis techniques need to be developed to make real-time, process analysis and control possible before the formation of harmful compounds. PAT has come a long way since then, with inline Raman spectroscopy, near infrared spectroscopy and mass spectrometry allowing for the continuous measurement of the reaction progression, thus enabling the timely intervention if any unwanted byproducts are formed (Bakeev, 2010). The FDA's PAT guidance of 2004 has made it easier for these methods to be adopted in the pharmaceutical production.

3.12 Inherently Safer Chemistry for Accident Prevention

Substances and their forms used in the chemical processes need to be chosen so as to ensure that the danger of chemical accidents, releases, explosions and fires is as low as possible. The Bhopal catastrophe of 1984, where the release of methyl isocyanate from the Union Carbide pesticide plant led to thousands of casualties and hundreds of thousands of injuries is the worst case ever known of chemical accidents arising from the storage of inherently hazardous intermediates in

huge amounts (Broughton, 2005). One way in which green chemistry deals with this problem is by taking into account if dangerous intermediates can be formed on-site and immediately used or if less hazardous reagents can be used instead of the more hazardous ones.

4. Metrics and Measurement in Green Chemistry

The application of green chemistry in practice requires quantifiable metrics allowing chemists to assess and compare different processes from the point of view of environmental friendliness and improve them accordingly. There is no such single metric and in most cases the set of them is used (Lapkin & Constable, 2008).

The E-factor, as noted, captures waste generation but says nothing about the nature of the waste, a process generating one kilogram of sodium chloride per kilogram of product is rated identically to one generating one kilogram of chromium hexavalent waste, though their environmental implications differ enormously. The environmental quotient (EQ), proposed by Sheldon, attempts to address this by multiplying the E-factor by an unfamiliarity quotient (Q) that reflects the hazard of the waste (Sheldon, 2007). Reaction mass efficiency (RME), developed by Curzons and colleagues, incorporates yield, atom economy, stoichiometry, and the mass of any solvent or reagent used, giving a more comprehensive picture of process efficiency (Curzons *et al.,* 2001).

Life cycle assessment (LCA) provides the most comprehensive framework, evaluating environmental impacts from raw material extraction through product manufacture, use, and end-of-life disposal or recycling. LCA studies of biobased chemicals have sometimes revealed that feedstock cultivation and processing carry significant environmental burdens of their own, land use change, water consumption, fertiliser runoff, that must be weighed against the benefits of avoiding fossil feedstocks (Pawelzik *et al.,* 2013). This complexity underscores the importance of systems-level thinking in green chemistry, lest improvements at one stage of a process be offset by worsened impacts at another.

The ACS Green Chemistry Institute's DOZN tool (Quantitative Green Chemistry Evaluator) takes yet another approach, scoring processes across twelve dimensions corresponding to the Twelve Principles and generating a visual profile that facilitates rapid comparison between alternatives (Roschangar *et al.,* 2018). Industrial adoption of such tools has been uneven but is growing, driven in part by the integration of green metrics into pharmaceutical regulatory submissions and supply chain sustainability reporting.

On the other hand, the ACS Green Chemistry Institute's DOZN tool (Quantitative Green Chemistry Evaluator) approaches this task, evaluating processes in terms of twelve criteria defined by the Twelve Principles and providing a visual image for easy comparison of the alternatives under consideration (Roschangar *et al.,* 2018). The spread of the use of similar tools is uneven across industry sectors, although their popularity is on the rise due to the inclusion of

'green indicators' into pharmaceutical regulatory submissions and sustainability assessments in supply chains.

5. Solvent Alternatives: A Case Study of the Progress of Green Chemistry

The search for greener solvents demonstrates both the goals and the challenges faced by green chemistry. Traditional organic solvents pose a number of dilemmas: they may be volatile, highly flammable and moreover toxic; their production requires energy and fossil resources; and their elimination or incineration results in the release of greenhouse gas emissions and air pollutants. However, solvents play a significant role in chemical processes, performing important functions in terms of the dissolution of reactants, heat and mass transfer and separation processes.

In the 1990-ies, supercriticAbove 31.1 °C and 73.8 bar, CO_2 goes supercritical and exhibits the properties of liquid while maintaining the ability of a gas to diffuse, and thus enables source extraction and reactions without toxic waste. Currently, supercritical CO_2 is used in coffee decaffeination as well as in dry-cleaning processes; pharmaceutical applications including the preparation of drug nanoparticles with the help of supercritical anti-solvent precipitation have been commercialized as well (Reverchon & Adami, 2006). Supercritical CO_2 is relatively non-polar and expensive for high-pressure equipment, and this is its main drawback.

Ionic liquids, salts that are liquid at or near room temperature, attracted enormous research interest in the 2000s as potential replacements for volatile organic solvents. Their negligible vapour pressure eliminates one important pathway for worker and environmental exposure. However, early enthusiasm was tempered by evidence that many ionic liquids are poorly biodegradable and acutely toxic to aquatic organisms; their synthesis often relies on halogenated precursors; and their high viscosity creates processing challenges (Pham *et al.,* 2010). More recent work on biodegradable protic ionic liquids and amino-acid-based ionic liquids addresses some of these concerns.

Deep eutectic solvents (DES), first described by Abbott and colleagues in 2003, have attracted growing attention as alternatives to ionic liquids. Formed by combining a hydrogen bond donor with a hydrogen bond acceptor, the classic example is a mixture of choline chloride and urea in a 1:2 molar ratio, DES exhibit many of the desirable properties of ionic liquids (low vapour pressure, tunable properties, wide liquid range) while being biodegradable, inexpensive, and often derived from natural compounds (Abbott *et al.,* 2003; Smith *et al.,* 2014). Applications in metal extraction, electrochemistry, organic synthesis, and pharmaceutical formulation have been demonstrated at laboratory and pilot scale.

Bio-sourced solvents coming from renewable sources belong to one of the biggest categories. 2-Methyltetrahydrofuran (2-MeTHF), which is processed from furfural, has been found as an alternative to tetrahydrofuran in pharmaceutical synthesis. Cyrene (dihydrolevoglucosenone), which is synthesized from cellulose, has a potential to replace dimethylformamide and N-

methyl-2-pyrrolidone (Sherwood *et al.,* 2014). Solketal, glycerol carbonate, and ethyl lactate which are all derived from biomass have been tested in different applications, although their effectiveness in the area of use is not as high as that of other solvents.

6. Catalysis: Enabling Greener Transformations

Catalysis is essential for green chemistry because catalysts lower activation energy and guide reactions through unique pathways; hence, bringing raw materials into a finished product with improved selectivity, low energy consumption and reduced waste. Today, it is possible to explore a large number of catalysis approaches – each of which has its own advantages under the green chemistry principles.

Enzymatic catalysis is referred to as biocatalysis, and this technology has changed significantly due to technology development in protein engineering and directed evolution. Enzymes work in mild aqueous conditions and provide unique selectivity including enantioselectivity, in addition to generating biodegradable proteins as waste. Frances Arnold received the Nobel Prize in Chemistry in 2018 due to her contribution in directed evolution of enzymes and showed how powerful lab evolution can be in tailoring enzyme properties as compared to the characteristics given by nature. For example, Merck used a transaminase enzyme that had been evolved through directed evolution for sitagliptin manufacturing (the compound contained in Januvia, the diabetes medicine) thereby replacing high-pressure rhodium-catalyzed asymmetric hydrogenation with millions of costs spent on the chiral auxiliary; in the end, the new method reduced waste by 19%, improved overall yield, and eliminated all heavy metals from the process, earning a Presidential Green Chemistry Challenge Award in 2010 (Savile *et al.,* 2010).

Photoredox catalysis, which utilizes visible light to perform single-electron transfer reactions with the assistance of excited-state metal compounds and photoactive organic chemicals, initiates new kinds of chemical reactions making it possible to carry out carbon-carbon bond formation under mild conditions and with excellent tolerance with functional groups (Prier *et al.,* 2013). The MacMillan research group at Princeton University has been particularly successful in using photoredox catalysis combined with organocatalysis in order to achieve two cycles of catalytic reactions aimed at creating complex organic molecules in a way that traditional thermal-based forms of chemistry fail. As photoredox reactions are carried out using light and not chemical oxidizing agents and/or reducing agents, it makes it possible to get rid of the necessity for using metals in an amount required when using traditional means of catalysis.

Heterogeneous catalytic processes which employ solids, mainly metal nanoparticles immobilized on porous materials, are one of the cornerstones of chemical production. The application of the nanotechnology in the world of chemistry has allowed the engineers to create special structures of catalytic reactants at the atomic level, which translates into increased conversion rates for some chemical processes in practice that are widely used in commercially important reactions.

Supported gold nanoparticles, for example, they can catalyse the low-temperature oxidation of carbon monoxide and the selective oxidation of alcohols under mild conditions, reactions that previously required toxic stoichiometric oxidants such as chromium(VI) or permanganate (Haruta, 2004).

7. Biorefineries, Renewable Feedstocks, and the Circular Economy

The transition from fossil-based to bio-based chemical production is one of the most ambitious challenges addressed by green chemistry. A biorefinery, analogous to a petroleum refinery, converts biomass into a spectrum of valuable chemicals and fuels. The U.S. Department of Energy's 2004 report 'Top Value-Added Chemicals from Biomass' identified twelve platform chemicals obtainable from sugar fermentation that could serve as starting materials for a large fraction of the existing petroleum-based chemical product tree (Werpy & Petersen, 2004). Subsequent work has refined and extended this list; succinic acid, for example, can be produced by fermentation of glucose and serves as a precursor to a range of polymers, pharmaceuticals, and food additives (Bozell & Petersen, 2010).

Lignocellulosic biomass, the structural material of plant cell walls, composed of cellulose, hemicellulose, and lignin, is the most abundant renewable organic resource on Earth, with annual production estimated at approximately 170–200 billion tonnes (Ragauskas *et al.,* 2014). Converting this complex, recalcitrant material into useful chemicals requires effective pretreatment, selective deconstruction, and efficient downstream conversion, each step presenting significant technical challenges. Ionic liquids and DES have been explored as media for cellulose dissolution and fractionation; biological saccharification using enzyme cocktails derived from wood-degrading fungi has been developed to commercial scale for bioethanol production; and catalytic hydrogenolysis routes to bio-based aromatic compounds from lignin are an active research frontier (Li *et al.,* 2015).

The circular economy, which refers to maintaining materials in usage as long as possible by employing recycling, remanufacturing and reuse principles, corresponds perfectly with the main concepts of green chemistry. Chemical recycling of plastics (the process of returning a type of polymeric waste to monomers or feedstock) is another approach to mechanical recycling that can be used for plastic stream which cannot be processed by mechanical recycling.

The concept of the circular economy, in which materials are kept in use for as long as possible through reuse, remanufacturing, and recycling, and waste from one process becomes feedstock for another, is closely aligned with green chemistry principles. Chemical recycling of plastics, which converts polymer waste back to monomers or feedstocks, offers an alternative to mechanical recycling for mixed or contaminated plastic streams that mechanical processes cannot handle. Glycolysis, hydrolysis, and pyrolysis routes for PET, polycarbonate, and polyurethane waste are being developed and commercialised by companies including Loop

Industries and PureCycle Technologies (Rahimi & García, 2017). Green chemistry principles inform the design of recyclable polymers: vitrimers, covalent adaptable networks that can be reprocessed like thermoplastics while retaining thermoset-like mechanical properties, exemplify molecular design in service of circular economy goals (Denissen *et al.,* 2016).

8. Industrial Applications and the Presidential Green Chemistry Challenge

The Presidential Green Chemistry Challenge Awards, administered by the EPA since 1996, provide a valuable empirical record of green chemistry in industrial practice. A review of award-winning technologies reveals several recurring themes: the replacement of stoichiometric metal oxidants with catalytic oxygen- or peroxide-based oxidation; the development of atom-economic catalytic routes to pharmaceuticals that displace multi-step synthesis sequences; the substitution of hazardous solvents with aqueous or bio-based alternatives; and the utilisation of enzymatic catalysis for the synthesis of chiral intermediates (EPA, 2021).

Among the most celebrated industrial achievements is the Dow Chemical Company's development of a catalytic process for producing propylene oxide using hydrogen peroxide (the HPPO process, jointly developed with BASF), which eliminates the chlorohydrin waste stream associated with the conventional chlorohydrin process and the large volumes of co-product generated by the Halcon/SM process; the new route reduces waste water by approximately 70–80% and eliminates chlorine use entirely (Trent, 2002). The HPPO plant at Antwerp has been in operation since 2008 and represents one of the largest implementations of green chemistry at industrial scale.

In the pharmaceutical sector, the development of Pfizer's atom-efficient synthesis of sertraline (the antidepressant marketed as Zoloft) replaced a three-step synthesis involving titanium tetrachloride, three solvents, and four recrystallisations with a single-step imine reduction in ethanol, reducing total waste by a factor of five (Dunn *et al.,* 2004). Similarly, the Sharpless epoxidation, a catalytic asymmetric epoxidation using tartrate esters as chiral ligands, recognised in the 2001 Nobel Prize, enabled the commercial synthesis of the anti-AIDS drug (–)-carbovir and numerous other pharmaceutical targets without stoichiometric metal oxidants.

Bio-based chemicals offer more examples of green chemistry applied on industrial scale. Braskem produced polyethylene from sugarcane ethanol known as 'I'm Green polyethylene' and prevents emission of about 2.5 tons of CO_2-equivalent per ton of polymer manufactured compared to traditional petrochemical polyethylene based on data from LCA commissioned by the company (Braskem, 2019). NatureWorks produces polylactic acid (PLA) from fermented glucose, which is commercially available biopolymer with a wide range of applications in textiles and packaging. Even though the Haber-Bosch process was important achievement of chemistry that requires large amount of energy (1-2% of global energy consumption), BASF is

conducting research of biological nitrogen fixation and electrocatalytic ammonia synthesis as greener alternatives (Guo *et al.,* 2019).

9. Challenges, Criticisms, and Unresolved Questions

Despite the great progress made by green chemistry as described above, there are still difficulties, technological, economic, institutional, and cultural, which the supporters of green chemistry are ready to admit.

In the scientific dimension, however, there's still a dilemma when it comes to balancing between greenness and efficiency. Thus, due to the different solvent properties, one cannot easily assume that greener solvents can replace conventional ones right away. Most biocatalysts are very selective, but they are often unstable and not sufficiently active and broad to be used in industry without being engineered properly. Likewise, it is quite probable that there are biobased platform chemicals that are not identical to their petroleum counterparts, which means another issue with downstream chemistry.To achieve a compromise solution, one needs to account for many green factors.

From an economic standpoint, it should not be assumed that going green equals instant financial advantages. Green innovations entail large investments, both in new technologies and in obtaining all permits necessary for proper operation of a green facility. The case of the chemical industry is particularly complex since it operates under great pressure, often utilizing body of already fully depreciated equipment. As a result, the industry is forced to bear both great expenses and low profits at the same time; hence, a lack of motivation for companies to make any changes in their processes due to existing regulatory frameworks that do not provide for pricing of environmental damages.

However, there are cultural and institutional obstacles in the field of chemistry. There are many countries where principles of green chemistry are either lightly touched or not addressed at all; additionally, there has always been an emphasis on novelty of method rather than efficiency and safety in the history of synthetic chemistry; hence, whenever a project fails to implement green innovations into the production cycle, this fact may not be reported at all, and no one learns from the experience gained (Figueiredo & Pato, 2000).

At long last, the limits of the green chemistry philosophy have been challenged. Some detractors contend that the traditional notion of the discipline restricts the focus too much on the chemistry and doesn’t pay enough attention to other components of the social and economic sphere, such as energy supply issues, land use, working conditions, and consumption patterns, which go beyond the lab of a chemist in the process (Mulvihill *et al.,* 2011). Newborn discipline of sustainable chemistry, understood as either an alternative to green chemistry or identical to it by various researchers, tries to widen the concept to include those systemic aspects as well.

10. Future Directions

The following stages of the development of the green chemistry discipline are likely to be determined by several borderlines. Electrocatalysis and electrochemical synthesis in the processes with the use of electrochemical means instead of chemical agents to initiate redox reactions give an opportunity for chemical production completely detached from the crude oil feedstock provided renewable energy is used. Electrochemical amination, C-H functionalisation, and CO_2 conversion into fuels and chemicals are constantly blooming fields (Yan *et al.,* 2017). The decreasing price for renewable electricity gives electrochemical methods more and more chances to compete against usual thermochemical processes.

Artificial intelligence and machine learning are changing how quickly and effectively chemicals can be discovered. Analytics that can use the chemistry literature to create predictive models of reactions, yields, and selectivity are starting to automate the process of finding synthetic routes in retrosynthetic analysis and determining reaction conditions and thus minimizing the need for experimentation. Using machine learning and high-throughput experimentation is helping with the rapid exploration of catalysts, solvents, and reagents over an area that would be impossible with empirical approaches.

Another frontier is the field of microbiomes and synthetic biology. Microorganisms can be modified to synthesize complicated molecules from simple material through the use of well-defined biosynthetic pathways. The production of artemisinin, a potent antimalarial drug previously extracted from the sweet wormwood plant, was engineered into Saccharomyces cerevisiae by the Keasling group at UC Berkeley, dramatically increasing supply and reducing cost (Ro *et al.,* 2006). Metabolic engineering of similar complexity is now being applied to a growing array of industrial chemicals, pharmaceuticals, and materials.

Flow chemistry and process intensification represent a more near-term but highly impactful frontier. Continuous flow reactors, which process material in a continuously moving stream rather than in batch vessels, offer improved heat and mass transfer, safer handling of reactive or hazardous intermediates (which never accumulate in large quantities), easier in-line monitoring, and direct scalability from laboratory to production scale (Plutschack *et al.,* 2017). The pharmaceutical industry has been an early adopter. Leading companies such as Eli Lilly, AstraZeneca, and Novartis have all published descriptions of flow chemistry technologies that have brought considerable gains in safety, yield, and waste minimization relative to classical batch procedures.

Conclusion

The field of green chemistry has achieved much in the quarter century since it has been formally introduced and defined. It has provided a coherent theoretical and philosophical basis for the practice of green chemistry, known as the Twelve Principles. It has developed a set of quantitative metrics that allow measuring, comparing, and monitoring environmental

performance. It has inspired a huge amount of scientific and industrial advances (in the areas of catalytic asymmetric synthesis, enzymatic processes, supercritical fluid technologies, and production of bio-based platform chemicals). Most importantly, green chemistry has started to transform industrial practices. A lot has to be done. The distance separating the expectations of the green chemistry and the actual state of chemical industry is immense. Therefore, fossil fuels hold a leading position, dangerous solvents are being used widely and the amount of wasted materials from pharmaceutical production has been decreased only slightly. To change the old habits of chemical industry, it is not enough to come up with ideas, it is necessary to make long-term investments, introduce enabling regulations and create a culture of constant improvement in the industry.

The problems primarily targeted by green chemistry are still pressing, such as depletion of resources, poisoning of the planet and deterioration of the environment. In fact, the issues in today's world may be even more crucial due to the current state of the environment and the rising level of climate change, pollution and synthetic chemicals. The future of the field is likely to be bright if it attracts the best specialists of the industry as soon as possible.

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DELETERIOUS EFFECTS OF SMARTPHONE RADIATIONS ON THE REPRODUCTIVE HEALTH OF MALES: A MINI-REVIEW

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Abstract

The global surge in smartphones, laptops, and 5G routers has raised concerns regarding electromagnetic radiation (EMR) and its impact on male reproductive health. Research from databases like PubMed indicates that chronic exposure to radiofrequency electromagnetic fields primarily impairs sperm parameters via two main biological mechanisms: scrotal hyperthermia and radiation-mediated oxidative stress. The thermal effects disrupt spermatogenesis which requires a temperature 2°C to 4°C cooler than core body temperature for continued sperm production. Storing mobile phones in front trouser pockets transfers heat and elevates testicular temperature, altering semen parameters. The non-thermal pathways trigger mitochondrial dysfunction, driving the overproduction of Reactive Oxygen Species (ROS). This resultant oxidative stress overwhelms cellular defences, damaging cell membranes and inducing sperm DNA fragmentation. The human and animal data demonstrate significant declines in sperm motility, viability, and structural integrity. The adverse reproductive outcomes are strongly tied to the duration of device usage and proximity to the device. The purpose of this mini-review aimed to assess the deleterious effects of smartphone radiations on the reproductive health of males.

Keywords: Smartphones, Oxidative Stress, Infertility, Spermatogenesis.

Introduction

There is an increase in the usage of mobile smartphones, notebooks, and wireless internet systems like Wi-Fi and 5G modems/routers throughout the world; these gadgets release a significant quantity of electromagnetic radiation (EMR) that may engage through the male reproductive system either via thermal or mechanisms that do not involve heat (Figure 1). The male reproductive system is among the biological systems most impacted, attributed to the sensitivity of the testes to temperature and radio-frequency electromagnetic radiation (RF-EMF). Normal spermatogenesis in testis requires a temperature 2°C to 4°C cooler than core body temperature for continued sperm production. Storing mobile phones in front trouser pockets transfers heat and elevates testicular temperature, altering semen parameters. Clinical and experimental research has documented how scrotal hyperthermia (elevated testicular

temperature) directly causes male subfertility and impaired sperm production. In human trials, healthy fertile men who underwent localized testicular warming in a 43°C water bath for 30 minutes daily over 10 consecutive days reached their lowest points in sperm concentration and motility six weeks after the heat exposure, experiencing an average 30% drop in concentration and a 65% drop in motility. In almost all human trials, sperm count, motility, and DNA integrity parameters naturally returned to healthy baselines within 8 to 12 weeks after the heat source was completely removed (1). Alterations in testicular tissue morphology, reduced sperm quantity, heightened mortality rates, compromised sperm DNA integrity, and elevated blood-brain barrier permeability, along with increased mitochondrial ROS generation, are regarded as unanticipated occurrences linked to exposure to radiations of smartphones, potentially contributing to male infertility due to oxidative stress. The purpose of this mini-review aimed to assess the deleterious effects of smartphone radiations on the reproductive health of males.

Literature Search and Methodology

Related research that documented the impacts of EMR from smartphones' impact on male reproductive health between 2003 and 2020 was assessed. The database of PubMed was utilized. The Subject Heading system was utilized to gather pertinent investigative studies from PubMed utilizing the subsequent keywords: smartphone and reproduction, electromagnetic radiation and male fertility, and radio waves and reproduction, genotoxicity and RFR exposure, male fertility and non-ionizing radiation, RFR induce male fertility, or radiofrequency radiation and DNA damage.

Animal and Human Experimentations

EMR could change male’s reproductive-hormonal processes through influencing testicular activities essential for testosterone (steroidogenesis) and sperm production (spermatogenesis). The majority of research carried out in this area has been derived from animal testing. The human testicle is extremely sensitive to radiation and heat. Brief exposure of male Wistar rats to mobile phone radiation resulted in a small reduction in serum testosterone levels and testicular mass (2). EMR caused a notable genotoxic impact on epididymal sperm cells (3).

Typical sperm specimens subjected to a laptop computer linked to Wi-Fi for 4 hours showed a notable decrease in sperm motility and an increase in sperm deoxyribonucleic acid (DNA) breakdown (4). Extended-term exposure to EMR, whether of high or low frequency, may impact the human male germ cell (5). Nevertheless, contact to EMR modified pituitary activity in rats (6). Continuous exposure to EMR influenced the Leydig and Sertoli cells in male rats, consequently impacting male fertility (7,8). There was a rise in free radicals and consequently oxidative pressure, reduction in sperm count, and reduction in mobility and viability in men who were subjected to EMR (9). Prolonged contact with mobile phone EMR could lead to decreases in serum testosterone levels (10). EMR modifies typical reproductive functions in male rats; the

same may happen in male humans subjected to RF-EMF over an extended duration (11,12). The internal systems of laptops and smartphones utilized by men frequently produces EMR. In a study conducted by Zalata et al. a total of 124 human semen samples were exposed to mobile phone EMR; there was a significant decrease in sperm motility, sperm linear velocity, sperm linearity index, and sperm acrosin activity, moreover, a significant increase in sperm DNA fragmentation was noticed in the semen samples to RF-EMF compared with standard samples (13).

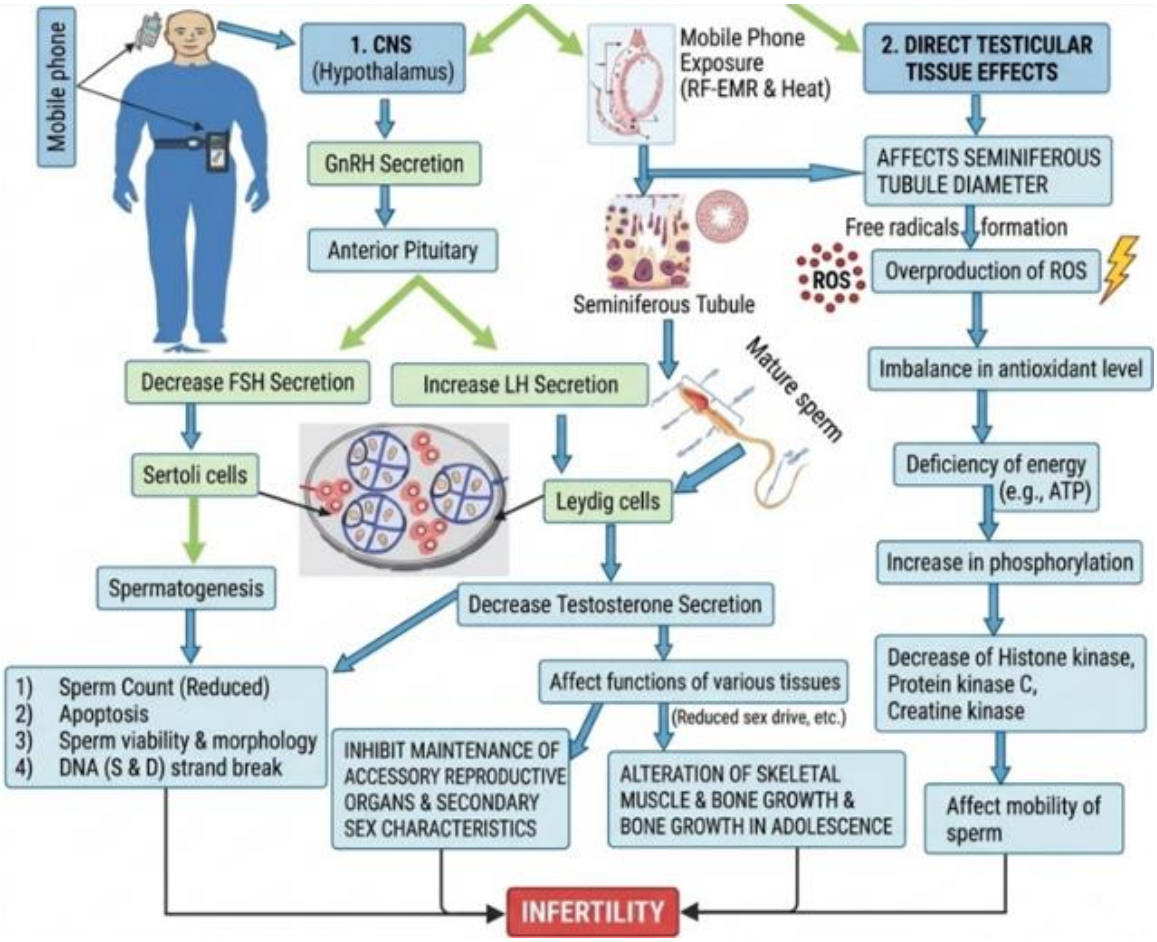


Figure 1: Effects of smartphones on the reproductive health of males

Discussion

The use of mobile phones has become a crucial aspect of our daily existence. Nonetheless, the impact of radiofrequency electromagnetic radiation (RF-EMR) produced by these devices on biological systems, particularly the reproductive systems, is presently a topic of lively discussion. Recent studies have demonstrated that radiofrequency (RF) radiation emanating from devices such as mobile phones and Wi-Fi may have adverse effects on male reproductive health. Leydig cells are responsible for production of major proportion of testosterone for supporting spermatogenesis in the testis under the stimulation of luteinizing hormone (14). Persistent mobile phone exposure was reported to decrease the serum testosterone levels affecting sexual differentiation of the fetus as well as male spermatogenesis (15,16). The proof regarding the

detrimental impacts of RF-EMF released by smartphones on male reproductive health remain unclear since the majority of the research conducted EMR exposure research was primarily carried out on rats. The global rise in smartphone usage has established locations for mobile phone base stations to be positioned in homes, educational institutions, and healthcare facilities. This has elevated public issues particularly regarding the newest 5th generation mobile communication technology (5G advancements), concerning the protection of residents subjected to radiation from those gadgets. Exposure to mobile phone EMR decreases sperm viability, motility, and sperm total antioxidant capacity in rats and results in oxidative stress (16). EMR exposure caused an injury in the blood–testis barrier and induced immune infertility in male mice (17). However, there is a need to conduct more investigations to determine the thermal and non-thermal effects of the 5G smartphones RF emissions on cell membrane structures and immune system (18).

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FROM BLACK-BOX MODELS TO TRANSPARENT DECISIONS: ADVANCES AND CHALLENGES IN EXPLAINABLE ARTIFICIAL INTELLIGENCE

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Abstract
The use of artificial intelligence (AI) systems to support decision making is increasingly being adopted in high-impact areas including health, finance, education and public. Using techniques from artificial intelligence, machine learning algorithms can identify patterns in large datasets but many do not predict (using a confidence measure) well. The lack of transparency has resulted in practical implications for accountability, bias, error detection and user confidence. Explainable AI, often abbreviated as XAI, refers to set of techniques aimed at making the behavior of a model more understandable so as to developers, domain experts, individuals as well as decision makers. The document is a narrative review for major XAI concepts, methods, challenges of evaluation, and application areas. The post covers interpretable models, SHAP, LIME, counterfactual explanations, example-based explanations, and other techniques to explain deep learning models and systems. The authors want to make sure that the theoretical work presented is credible. No explanation method is appropriate for all models, tasks or audiences finds the paper. If a model explanation does not consistently reflect model behavior, is unstable to minor changes in input, or is taken to be evidence of causality, then it is misleading. Therefore, XAI should be seen as one part of a larger assurance process, incorporating data governance, performance evaluation, fairness, robustness, human oversight and continual monitoring. the paper suggests some avenues of research in standardized evaluation, human-centered explanation design, multimodal systems, generative AI, privacy, and context-sensitive validation.

Keywords: Explainable Artificial Intelligence, XAI, Interpretability, Model Transparency, SHAP, LIME, Explanation Fidelity, Responsible AI.

1. Introduction

Artificial intelligence was born as a niche research topic and soon morphed into systems affecting everyday choices. Machine-learning algorithms classify medical images, assess financial risk, recommend educational content, detect suspicious transactions, prioritise information and help with operational planning. A straightforward forecast is often inadequate. In the healthcare context, the assignment assesses a health care provider's need to understand what evidence informed a risk assessment. For a financial institution, the justification for a lending decision is the priority, while a software engineer wishes to understand why a model

behaves differently across demographic groups. The need for explainable artificial intelligence (XAI) has exploded.

The expression black box refers to a model whose inner workings are hard to verify or describe, especially if it incorporates many parameters or complicated interactions. Although deep neural networks and large ensembles can extract useful patterns from data, their predictive power does not imply we understand their reasoning. For that reason, stakeholders may find it difficult to identify errors, dispute a forecast or know when to trust a machine-generated result.

XAI is composed of more than one algorithm. This includes building interpretable models, explaining post-hoc, evaluating explanations, and investigating people's understanding of explanations, and many more. It covers much ground. Doshi-Velez and Kim (2017) argued in favour of a more scientific definition of interpretability. Lipton (2018) stressed the importance of clarifying the intended meaning of the term by researchers. Subsequent evaluation classified XAI mechanisms based on model dependence, scope, explanation format, and audience (Guidotti *et al.,* 2018; Arrieta *et al.,* 2020).

This paper critiques existing XAI approaches and their shortcomings. A proposal for a new algorithm or a new experimental dataset is not made. The major literature is instead reviewed with issues which should guide the choice and assessment of explanatory techniques.

2. Review Method and Scope

We reviewed the key papers, highly cited methodological papers, review articles, and particular standards or guidance documents to illuminate the development of XAI and major technical conversations. The assessment is organized according to interpretability principles, explanation techniques, evaluation standards, application areas and open research issues through thematic sets. The cited works include early studies on interpretable models and local explanations, later studies on feature attribution and counterfactual explanations, as well as studies on the reliability of explanations and on their human use.

The method was used to write a structured summary, not a reproducing systematic review. Not all publications in the area are claimed to be obtained or reviewed. A pending systematic review will reinforce the evidential basis through the specification of databases and search queries, inclusion/exclusion criteria, method of screening, and a well-structured quality-assessment framework.

3. Conceptual Foundations of Explainable AI

3.1 Interpretability and Explainability

Interpretability is often defined as the ability of a person to understand the model's structure or actions, while explainability is often defined as the ability of techniques to provide explanations or reasons for a specific prediction or the model's overall behaviour. There's some overlap between the definitions and scholars don't use them interchangeably. A simple decision tree is

easy to inspect, while a complex neural network may need a different way of explaining. The distinction is useful, but it should not be interpreted as a strict definition.

3.2 Intrinsic and Post-Hoc Approaches

Intrinsic interpretability is achieved by building models whose structure is relatively simple to inspect. Linear models, sparse models, rule lists and compact decision tree models are examples. Post-hoc explainability is applied after a model has been trained and provides explanations for its predictions or actions. Post-hoc techniques can be used for sophisticated models. The explanation is an ancillary illustration and may not fully capture the initial model. Rudin (2019) warns that in high-stakes settings, researchers must ask themselves if an interpretable model can achieve the performance required before trusting the explanations of a black-box model.

3.3 Global and Local Explanations

A global explanation attempts to explain global model behaviour. And the features that influence predictions across the whole dataset. A localized explanation points to a specific prediction or a small region of the input domain. Each view can be useful, but they answer different questions. A global feature ranking may not explain why an individual has a high risk score, while a local explanation may not reveal patterns that hold across a population.

4. Major Explainability Methods

4.1 Feature Importance and Permutation Methods

Feature importance methods quantify the contribution of input variables to the efficacy of the model or to the predictions. Permutation importance estimates the change in model performance when the values in a feature are shuffled. It is applicable to different model types. Correlated features can make it less interpretable though, as some information between variables may be substituted with other features. Thus, importance scores should be viewed as model and data dependent evidence rather than as definitive proof of a feature's causal effect on an outcome.

4.2 LIME: Local Surrogate Explanations

Local Interpretable Model-agnostic Explanations (LIME) explain an individual prediction by generating new perturbed instances around the original instance, querying the original model and creating an interpretable model to approximate the original model's behaviour in the close locality of the instance (Ribeiro *et al.,* 2016). For instance, if a classifier classifies a transaction as suspicious, LIME could identify the features that contributed most to this transaction. The approach is flexible but the results may depend on the sample generation, the features that are perturbed and the choice of the locality kernel or other design parameters. A plausible sounding explanation does not necessarily mean a correct explanation.

4.3 SHAP: Shapley-Value Feature Attribution

SHAPley Additive exPlanations (SHAP) links feature attribution to the Shapley values from cooperative game theory. It attributes contributions to features relative to a baseline prediction. It

offers a unifying framework for local explanations which can be aggregated for global explanations (Lundberg & Lee, 2017). TreeSHAP offers efficient calculations for tree-based models, and KernelSHAP approximates Shapley values for a broader range of model classes. SHAP is popular because the attribution framework has nice theoretical properties. However, the results still depend on the background distribution, assumptions about feature dependence, and the questions asked. The attribution values should not be interpreted as causal influences.

4.4 Counterfactual Explanations

A counterfactual explanation describes a change to an input that would lead to a different model output. For instance, a system can indicate that a predicted outcome would be different if a certain qualifying attribute was altered. Wachter *et al.,* (2017) played a crucial role in legitimising counterfactual explanations as a method for explaining automated decisions. Counterfactuals must be credible, actionable if possible and respect domain constraints. They should not suggest changes that can't be done, reveal private information or suggest that a person can change things that realistically can't be changed.

4.5 Example-Based and Prototype Explanations

Methods based on examples explain a prediction by showing representative examples, similar examples, prototypes or important training examples. Such elucidations might be intuitive, for people infer through analogies. However, similarity is representation and distance metric dependent and an analogue may not be relevant in the way a user expects. Explanations may disclose information from training records, which raises privacy and data protection concerns.

4.6 Explainability for Deep-Learning Models

The various explanations of deep learning contain saliency maps, attention visualisations, gradient-based attributions, LRP, concept-driven approaches and text-based explanations. These techniques can identify areas of an image, input tokens, or internal representations associated with a prediction. However, credibility in visuals alone is not enough to be trustworthy. According to a recent research, Adebayo *et al.,* (2018), it shows that some explanations may not depend much on the parameters of trained models or the training dataset. Thus it proves the need of sanity check for saliency techniques. Explanation methodologies are not to be accepted as valid on the basis of superficiality.

5. Conceptual Framework for XAI

A complete workflow for the responsible use of explanations is shown in Figure 1. Explanations are generated after model training and prediction. But the process should not stop after an explanation is generated. Explanations need to be assessed in context. Based on evaluation results and user input, modifications to data, model architecture, explanatory parameters or operational protocols may be necessary.

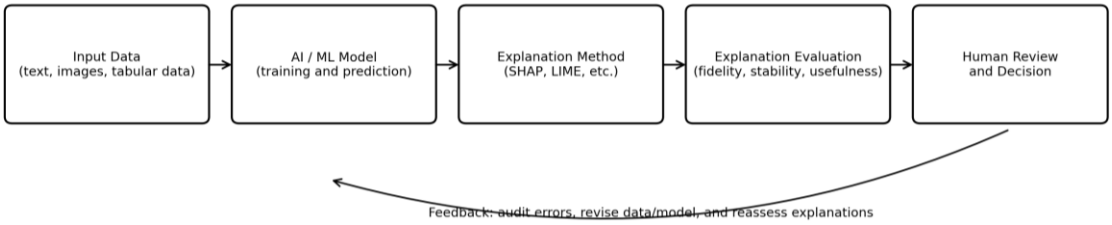


Figure 1: Conceptual workflow for explainable artificial intelligence.

6. Comparison of Common Xai Methods

Method	Typical Purpose	Strengths	Key Limitations
Interpretable models	Understand model structure directly	Transparent logic; often easier to audit	May not capture complex patterns; complexity can reduce clarity
Permutation importance	Assess global feature reliance	Model-agnostic and conceptually simple	Correlated features and metric choice can distort interpretation
LIME	Explain one prediction locally	Flexible across model types	Sensitive to perturbation and locality choices
SHAP	Attribute prediction to features	Consistent attribution framework; local and global use	Computational cost and background/dependence assumptions
Counterfactuals	Show input changes linked to a different output	Can be actionable and user-oriented	May be infeasible, unstable, or mistaken for causal advice
Saliency / relevance	Highlight input regions or tokens	Useful for image and text models	Visual appeal does not guarantee faithfulness
Example-based methods	Explain through similar or representative cases	Often intuitive to users	Depends on similarity metric; possible privacy risks

7. Evaluating Explanation Quality

7.1 Fidelity and Faithfulness

Faithfulness refers to how well the explanation replicates representative model behaviour. For example, a local surrogate should closely resemble the original model in the local region it is intended to explain. A transparent yet incorrect explanation of the model may be worse than no explanation at all; it may create a false sense of security.

7.2 Stability and Robustness

This stability question asks whether the same or similar input slightly changes the interpretation or not. The basic behavior of the model is unchanged. A large variation in explanation for a small change in input might not be necessarily reliable. Robustness evaluations should check the

sensitivity to perturbations, background samples, random seeds and relevant methodological settings.

7.3 Comprehensibility and Usefulness

Technical accuracy differs from the usefulness of explanation to an individual. While the mathematical explanation may be precise, it is often too sophisticated for patients, clients, students, or public sector individuals. The audience's level of understanding of things, the impact of the decision and a specified action that the explanation tries to help the audience carry out are key things to consider. When humans assess the model, we can discern whether users understand the explanation, accept the limits of the model, and leverage better decision-making.

7.4 Fairness, Privacy, and Security

Clarifications assist auditors in comprehending differences in treatment; however, this does not mean that the treatment is confirmed to be equitable. The definition and metrics for equity need to be conceptually precise but contextually relevant. Exposing sensitive properties or data information is also the risk of clarification. Misleading impressions can be created using explanatory interfaces. As shown by Slack *et al.,* in 2020, explanation methods can be vulnerable to adversarial attack; thus, we must test explanation system instead of assuming they are trustworthy.

8. Applications of Explainable AI

8.1 Healthcare

In the healthcare field, XAI is able to help clinicians evaluate predictions of disease risk, medical imaging, patient deterioration or treatment outcomes. An explanation can draw attention to salient features or regions of an image, but it should not substitute for clinical judgement or make a diagnosis on its own. Validation on representative cohorts, attention to data leakage and distribution changes, and careful assessment of the influence of explanations on clinical decisions are all required for application of the application in clinical settings (Tjoa & Guan, 2021).

8.2 Finance and Insurance

Financial institutions use predictive algorithms to detect fraud, assess credit risk, process claims and perform anti-money laundering assessments. Clarifications can help internal auditing and allow decisions to be discussed. However, the explanation methods should be evaluated for consistency and should not make systems vulnerable to manipulation or disclose confidential information. A rationale produced after a decision is not necessarily a legally valid or factually correct justification.

8.3 Education

Education analytics can warn students when they are predicted to have any academic trouble. Clarifications enable educators to understand which observed factors influenced a forecast.

Systems of this nature should refrain from generating deterministic classifications of students. They should acknowledge the contextual and measurement constraints. Moreover, predictions should serve to expand, rather than limit, educational opportunities.

8.4 Cybersecurity and Public Services

Explanations pertaining to security can enable analysts to investigate alerts, suspicious activity or discovered anomalies. They could help to assess decisions on eligibility or resource distribution in the public service space. Applications of these kinds usually involve high stakes, sensitive data, and evolving attackers. XAI must always be supported by human oversight, secure recording, self-diagnosis and a means for contesting choices.

8.5 Natural Language Processing and Generative AI

For language models, an explanation can be identifying important parts of the input, finding supporting evidence, explaining the limits of the model, or separating generated claims from facts. A coherent natural-language explanation can also be persuasive, even if it is not faithful to the computation that produced the response. Where possible, systems should provide evidence that can be verified and distinguish between a rationale generated by the model and an explanation that has been independently verified.

9. Major Challenges and Research Gaps

First, there is no common evaluation measure in the domain that captures all important aspects of an explanation. There are distinct worries about fidelity, stability, simplicity, usefulness and fairness, and increasing one might degrade another. Second, elucidations are context dependent: the elucidation that would be most useful to the model creator may not be useful to the domain specialist or affected person. The relationship between explanation and trust is complicated. A clarification may increase confidence, but not the user's ability to find errors. Thus researchers should study calibrated reliance, especially when users know when to disregard a model.

Fourth, many explanation approaches are sensitive to modelling assumptions, data distributions and implementation details. Fifth, feature attribution can be misconstrued as causal inference, which is a potential pitfall. Attribution can show how a model uses features, without showing that changing a feature would change the real world outcome. Sixth, explanatory techniques could be subject to distortion or could reveal confidential data. Seventh, the rapid growth of multimodal and generative AI raises new questions about explanations across text, images, audio, and structured data and how to trace evidence through sophisticated pipelines.

Another difference is the realistic assessment of XAI in actual workflows. Benchmark scores can neither confirm nor deny that better explanations improve professional judgement, make the contestability process more effective, reduce error, or create undue dependence. More fieldwork and deliberate user experiment design are needed. To enhance the reproducibility of our findings,

investigators should disclose explanatory variables, data assumptions, model specifications, and limitations.

10. Future Research Directions

Going forward, more research should be done on developing assessment methods that integrate technical assessments with human. Tests should assess consistency, stability, sensitivity to attention-inducing features, and effectiveness on sub-populations; user studies should assess understanding and confidence. By using traditional reporting methods, we can improve reproducibility and comparability.

One more method is context response explanation. Systems should tailor the level of explanation to the user's role, expertise, and decision-making authority while maintaining the underlying evidence. Investigations must adopt causal and counterfactual approaches that are clear about their assumptions and segregate model behavior from true causal claims.

On a large scale, the XAI has to be embedded in larger governance. This encompasses data documentation, model cards, privacy protections, bias assessments, robustness assessments, versioning, incident documentation, and human review or appeals processes. We need to think through source attribution, traceability of evidence, and being distinct between a "compelling" explanation, and a "validated" explanation when using generative AI and multimodal systems

11. Discussion

From the literature explanation, it is better to view explainability as a set of techniques and practices, rather than as an intrinsic property that makes an AI system reliable per se. Inherently interpretable models can provide immediate insight into the decision making process, provided they are appropriately complex and predictive enough. The models and their fit/accuracy after the model have been expanded. SHAP and LIME are useful and popular models, but neither can be considered strictly superior. On Counterfactuals and Example-based Explications may be more convenient for some audiences, but require careful scrutiny for feasibility, privacy and deception issues.

An accountable XAI process begins with a specific question: who needs the explanation, what will it support a decision on, and what would evidence for sufficiency look like? The selected method should align with the model, the nature of data, the potential risks and the targeted audience. In the end, explanations should be evaluated in terms of model performance, fairness, safety, and feasibility. For this reason, we do not assume that transparency alone will resolve the larger issues of accountable AI.

Conclusion

To make accurate predictions alone may not suffice to address real-life dilemmas in decision making. This is why research in explainable artificial intelligence is gaining traction. Various Strategies of XAI: Interpretable Models, Feature Attribution, Local Surrogates, Counterfactuals,

Example-driven Methods, Deep-learning Visualisation. Every approach asks different questions and has restrictions. Options when deciding how to explain things; fidelity, stability, clarity, context and audience needs. We should not interpret an explanation as a narrative causation or promise of fairness or evidence for the reliability of the model. Developing XAI further will need better validation, user evaluation, replicable documentation, integration into a wider umbrella of AI governance. The goal should not only be transparency, but also explanations that are scientifically reasonable and that facilitate wise decision-making or actions.

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INTEGRATING TECHNOLOGICAL INNOVATION AND ADAPTIVE PATHWAYS TOWARD CLIMATE-SMART FOOD SYSTEMS

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Abstract

Global agriculture faces converging pressures from climate change, resource degradation, demographic growth, and geopolitical instability that threaten food security for a projected 9.7 billion people by 2050. Conventional intensification has reached diminishing returns and often exacerbates environmental harm. This paper synthesizes recent advances (2020–2026) to argue that reinventing agriculture requires the deliberate integration of technological innovation with resilience principles across production, value chains, and governance. Key domains examined include artificial intelligence–driven precision systems, gene editing and multi-omics approaches, climate-smart and regenerative practices, controlled-environment agriculture, and systems-level digital twins and policy frameworks. Evidence from reviews and institutional reports indicates substantial gains in resource efficiency (water savings up to 30%, pesticide reductions exceeding 90% in targeted applications, yield stability under stress) when innovations are contextually adapted and inclusively scaled. Persistent barriers—data inequities, high upfront costs for smallholders, limited model generalizability, and policy fragmentation—create a "climate resilience divide." The paper advances an integrated framework linking cross-domain technologies, whole-chain interventions, and multi-scale governance, and concludes with priority research, investment, and policy recommendations for transformative, equitable resilience.

Keywords: Climate-Smart Agriculture, Precision Agriculture, Artificial Intelligence, Agricultural Resilience, Gene Editing, Digital Twins, Agri Food Systems Transformation.

1. Introduction

Agriculture stands at an inflection point. Rising temperatures, shifting precipitation patterns, more frequent extremes, soil degradation, biodiversity loss, and water scarcity are already reducing yields of staple crops in many regions, with projections of further declines (for example, maize yield reductions of up to 24% in vulnerable areas under high-emissions pathways by 2030). Simultaneously, agriculture remains a major contributor to greenhouse-gas emissions, deforestation, and freshwater withdrawals. The dual imperative—to produce more nutritious food with fewer environmental impacts while building adaptive capacity—cannot be

met by incremental improvements alone. "Reinventing agriculture" therefore means moving beyond productivity-centric paradigms toward systems that are simultaneously productive, adaptive, and mitigative. Resilience here is understood as the capacity of agrifood systems to absorb shocks, adapt to changing conditions, and transform when necessary, while maintaining core functions of food provision, livelihoods, and ecosystem services. Innovation—technological, institutional, and social—is the primary lever for this reinvention.

This paper reviews and synthesizes evidence on how frontier and near-term innovations can enhance resilience. It draws on recent peer-reviewed reviews, World Economic Forum deep-tech analyses, FAO road maps on digital agriculture and AI, and assessments of climate-smart practices. The objective is to provide a coherent, innovation-oriented perspective suitable for an international journal audience of researchers, policymakers, and practitioners.

2. Conceptual Framework: Innovation–Resilience Nexus

Resilience in agrifood systems operates at multiple scales (field, farm, landscape, value chain, national, global) and encompasses ecological, social, and economic dimensions. Innovation contributes by:

- Increasing buffering capacity (e.g., drought-tolerant varieties, diversified systems)
- Enabling rapid sensing and response (real-time monitoring, predictive analytics)
- Facilitating transformation (new production paradigms such as vertical farming or regenerative transitions)
- Improving inclusivity and equity so that resilience benefits are widely shared.

Climate-smart agriculture (CSA) provides a useful organizing triad—sustainably increasing productivity, enhancing adaptation/resilience, and reducing or removing greenhouse-gas emissions—while recognizing trade-offs that must be managed contextually. Deep-tech convergences (AI + robotics + sensing + biotechnology + nanotechnology) amplify these outcomes when embedded in enabling ecosystems of data infrastructure, skills, finance, and policy.

3. Methodology

This is a narrative synthesis informed by systematic elements. Literature published primarily between 2020 and 2026 was examined, prioritizing high-quality reviews on AI applications in agriculture, climate-smart practices, deep-tech in agrifood systems, and institutional reports from FAO, World Economic Forum, IFPRI, and related bodies. Search domains included precision agriculture, gene editing for stress resilience, digital twins, regenerative approaches, and barriers to scaling. Emphasis was placed on empirical performance metrics (resource savings, yield stability, emission reductions) and documented limitations (generalizability, equity, multi-season validation). The synthesis identifies convergent findings, knowledge gaps, and actionable pathways rather than performing a formal meta-analysis.

4. Key Innovation Domains

4.1 Artificial Intelligence–Driven Precision and Digital Agriculture

AI, machine learning (including hybrid CNN-LSTM models), computer vision, IoT sensor networks, drones, and robotics enable site-specific management. Documented benefits include improved yield prediction across space and time, earlier disease and pest detection (often weeks ahead of visual scouting), optimized irrigation (water savings reported up to 30%), and substantial reductions in nitrogen and pesticide use. Reinforcement learning shows promise for adaptive irrigation under weather uncertainty. Digital twins at farm and watershed scales allow scenario testing of adaptation strategies before field deployment. Emerging tools such as foundation models, multimodal AI, and retrieval-augmented generation support decision support systems accessible via simple interfaces.

These technologies shift agriculture from reactive to predictive and from uniform to variable-rate management, directly strengthening resilience to climate variability.

4.2 Biotechnology, Multi-Omics, and Genetic Innovation

CRISPR and related gene-editing tools, combined with AI-assisted multi-omics and high-throughput phenotyping, accelerate development of climate-resilient and nutrient-enriched varieties. Advances include enhanced drought and heat tolerance, pest resistance, improved nutrient bioavailability (e.g., iron and zinc), and reduced anti-nutritional compounds. Synthetic biology approaches are producing microbial biofertilizers and biopesticides that lower chemical dependence. These genetic innovations provide intrinsic buffering capacity that complements management practices.

4.3 Climate-Smart, Regenerative, and Agroecological Practices

Conservation agriculture, agroforestry, diversified cropping, improved water and nutrient management, and soil-carbon-enhancing practices form the ecological foundation of resilience. When integrated with digital tools, they deliver measurable gains in productivity, income stability, dietary diversity, and emission reductions. Regenerative approaches restore soil health and biodiversity, increasing system buffering against extremes. Context-specific combinations (rather than universal packages) are essential.

4.4 Controlled-Environment and Alternative Production Systems

Vertical farming and other controlled-environment agriculture systems achieve dramatically higher yields per unit land and water (often 10–20× with 95% less water in optimized setups) and enable year-round production independent of outdoor climate extremes. Integration of AI for environmental control and renewable energy (agrivoltaics, on-farm biogas) further enhances sustainability. Alternative proteins and advanced aquaculture systems reduce pressure on land and water resources.

4.5 Systems Integration, Supply Chains, and Governance

Block chain for traceability, digital platforms for market access and advisory services, and whole-value-chain approaches extend resilience beyond the farm gate. Policy and institutional innovation—targeted spatial intelligence for interventions, inclusive R&D, and blended finance—are required to scale solutions equitably. FAO digital agriculture and AI roadmaps and similar frameworks emphasize interoperable, trusted, and locally adaptable ecosystems.

5. Challenges and the Climate Resilience Divide

Despite demonstrated potential, adoption remains uneven. High capital and data requirements favor large-scale operations; models trained in data-rich environments often fail to generalize to smallholder contexts (spatial overfitting); interpretability and multi-season validation remain limited; rural connectivity, skills gaps, and regulatory uncertainty constrain uptake; and power imbalances in data and technology ownership risk exacerbating inequities. These factors constitute a structural climate resilience divide that innovation alone cannot close without deliberate equity-oriented design and investment.

6. Pathways for Scaling and Transformation

An integrated framework is proposed that coordinates three axes:

- Cross-domain integration (agronomy, AI, biotechnology, social sciences, policy)
- Whole-chain coverage (production through consumption and circularity)
- Multi-scale action (field to global), operating through iterative cycles of shared goals, diagnosis, co-design, intervention, monitoring, and adaptive feedback.

Priority actions include: long-term investment in participatory, gender-responsive R&D; open and interoperable data infrastructures with transfer-learning approaches for data-scarce regions; blended finance and risk-sharing mechanisms tailored to smallholders; skills development and digital literacy programs; and policy coherence that rewards resilience outcomes rather than solely production volume.

7. Discussion

The evidence consistently shows that technological innovation multiplies the effectiveness of ecological and management practices when deployed within supportive institutions. Isolated pilots, however, rarely transform systems. The greatest leverage lies in convergence—AI amplifying breeding and precision management, regenerative practices providing the biological substrate for digital optimization, and governance ensuring benefits reach the most vulnerable. Trade-offs (e.g., automation versus rural employment, data privacy versus model performance) must be explicitly managed. Future research should prioritize multi-season, multi-location validation; explainable and physics-informed AI; socio-technical evaluation of equity impacts; and foresight on emerging deep-tech combinations.

Conclusion and Recommendations

Reinventing agriculture for resilience is both necessary and feasible. By systematically integrating AI-enabled precision systems, advanced biotechnology, climate-smart and regenerative practices, controlled-environment solutions, and enabling governance, agrifood systems can simultaneously enhance productivity, adaptive capacity, and environmental performance. Success depends on closing the resilience divide through inclusive design, sustained investment, and adaptive institutions.

Recommendations for research communities, funders, and policymakers include:

- Prioritize hybrid models and digital twins with rigorous multi-season testing.
- Invest in open data platforms and capacity building targeted at smallholders and women.
- Align public and private finance with measurable resilience and equity metrics.
- Foster multi-stakeholder innovation ecosystems that move from pilots to scaled, context-adapted solutions.
- Embed continuous learning and foresight so that innovation remains responsive to evolving climate and societal needs.

Only through such deliberate, systems-oriented reinvention can agriculture fulfill its dual role of feeding humanity and safeguarding the planet under intensifying pressures.

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REGENERATED CELLULOSE FOR FLEXIBLE AND GREEN ELECTRONICS

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Abstract
The rapid expansion of portable, wearable and connected electronic technologies has increased the need for materials that combine reliable performance with lower environmental impact. Regenerated cellulose (RC), produced by dissolving natural cellulose and subsequently regenerating it into films, fibres, membranes, or porous structures, is a promising platform for sustainable electronics. Its renewable origin, hydroxyl-rich chemistry, hierarchical structure, mechanical flexibility and potential for biodegradation make it attractive as a substrate, separator, dielectric, or functional composite matrix. However, native cellulose is electrically insulating, hydrophilic, and difficult to process in conventional solvents; consequently, dissolution chemistry, regeneration conditions and interface engineering strongly determine the final properties. This brief review outlines the structure and processing of RC, summarizes direct functionalization and hybrid-composite strategies, and discusses its use in sensors, actuators, circuits, energy harvesting and storage, and electromagnetic-interference shielding.

Keywords: Regenerated Cellulose, Sustainable Electronics, Flexible Devices, Cellulose Composites, Sensors, Energy Storage, Biodegradability.

1. Introduction

Electronic products increasingly rely on flexible substrates, lightweight packaging, conformable sensors, and compact energy-storage components. At the same time, short product lifetimes and the accumulation of electronic waste have intensified interest in renewable materials and circular design. Conventional polymers and metal-rich components can offer excellent performance, but their feedstocks, processing requirements, and disposal pathways may create environmental burdens. Cellulose, the principal structural polysaccharide in plant biomass, offers an abundant renewable alternative. Yet the use of unmodified cellulose in electronics is limited by its insolubility in water and many common solvents, its sensitivity to humidity, and its intrinsically low electrical conductivity.

Regenerated cellulose addresses some processing limitations by temporarily disrupting the native cellulose structure through dissolution and then forming a new solid network during regeneration. The resulting material can be shaped into transparent films, membranes, fibres, gels, and porous architectures. Wang *et al.* recently reviewed this emerging field, emphasizing molecular structure, dissolution and regeneration mechanisms, functionalization, hybridization,

property engineering and applications across electronic-device classes [1]. The present brief review distils these themes and places particular emphasis on the relationships between processing, structure, performance, and environmental claims.

2. Molecular Structure and Regeneration

Cellulose consists of β-(1→4)-linked anhydro-D-glucose units. Numerous hydroxyl groups form intra- and intermolecular hydrogen bonds, contributing to chain association, crystallinity, and mechanical integrity. Native cellulose contains ordered and less ordered regions, and its multiscale structure extends from molecular chains to microfibrils and larger fibres. These features support strength and dimensional stability, but strong interchain interactions make cellulose difficult to dissolve without specialized solvent systems [2].

During regeneration, cellulose chains re-associate as the solvent environment changes. The solvent, coagulation bath, temperature, concentration, and drying conditions influence chain packing, pore structure, crystallinity, surface roughness, and optical properties. A dense regenerated film may provide good barrier performance and mechanical integrity, whereas a porous or gel-like structure can offer high surface area and pathways for electrolyte transport. Thus, regeneration is not simply a shaping step: it is a structure-control strategy. Reproducibility requires control of the complete process, including washing, residual-solvent removal, and drying.

Solvent selection is central to sustainability. A technically effective solvent is not automatically environmentally benign; toxicity, energy demand, solvent recovery, water use, and compatibility with large-scale equipment must also be considered. A credible process should demonstrate solvent recycling and quantify material yield and waste streams. These considerations are essential if RC is to provide a real environmental advantage over established polymer films.

3. Functionalization and Composite Design

RC is generally electrically insulating, so electronic functions are introduced through chemical modification, surface treatment, or hybridization with active materials. Direct modification can alter hydroxyl groups, surface charge, wettability, crosslink density, or interfacial adhesion. Such changes can improve water resistance, dimensional stability, mechanical toughness, or compatibility with subsequently deposited functional layers. Modification must be selected carefully because excessive crosslinking or chemical substitution may reduce flexibility, transparency, or biodegradability [3]. Figure 1 shows the regenerated cellulose (RC) membrane.

Hybridization combines RC with conductive, semiconductive, dielectric, magnetic, or electrochemically active components. Conductive networks may be formed using carbon-based materials, conductive polymers, or metallic nanostructures. Semiconducting particles and polymers can provide photoresponsive or charge-transport functions, while insulating fillers and coatings can tune dielectric behaviour and protect active layers. The cellulose network serves as

a mechanically supportive scaffold and can help distribute functional particles, but the electrical response depends on filler loading, dispersion, percolation pathways, and contact resistance [5].

Interfacial engineering is especially important. Poor adhesion between cellulose and a conductive phase can cause cracking, delamination, or unstable electrical signals during bending. Conversely, strong interfacial bonding and a well-connected network can improve durability. Increasing filler content may raise conductivity or shielding effectiveness, but can also increase stiffness, reduce optical transparency, and complicate recycling. The most suitable composite is therefore application-specific rather than universally optimal.

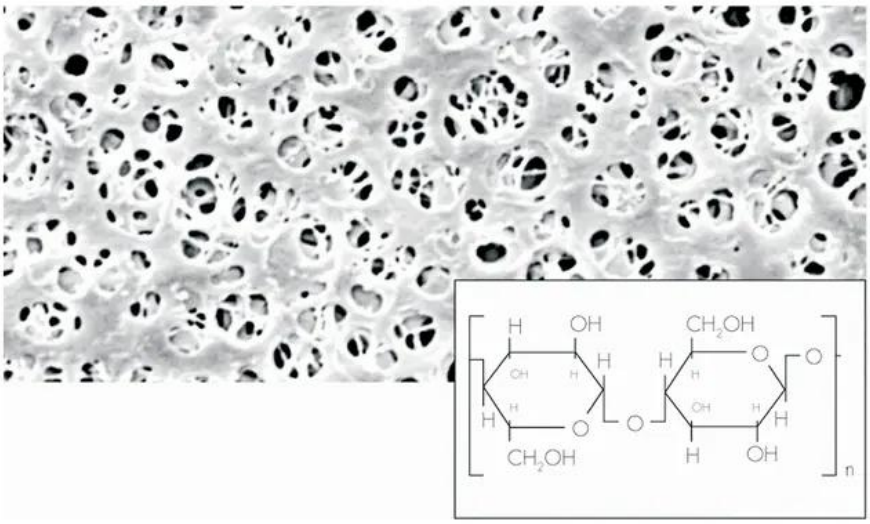


Figure 1: Regenerated cellulose (RC) Membrane [4]

4. Engineering the Key Properties

Mechanical strength and flexibility are controlled by cellulose concentration, regeneration history, orientation, porosity, plasticization, and crosslinking. Dense films can be robust but may be less compliant; porous materials can deform more readily but may have lower tensile strength. Multilayer designs and reinforcing networks can improve performance, although added components may reduce the simplicity of the material system [6].

Electrical conductivity is often governed by the continuity of the conductive phase rather than the cellulose itself. Percolating networks can enable charge transport at relatively low filler fractions, provided that contacts remain stable during strain and humidity changes. Optical transparency is similarly a structural outcome: uniform thin films and nanoscale dispersions may preserve transparency, while aggregates, pores, or thick conductive layers scatter or absorb light. Since cellulose contains abundant hydroxyl groups, water uptake can alter dimensions, dielectric response, ion transport, and sensor baselines. Protective coatings, hydrophobic modification, encapsulation, and humidity-aware calibration can mitigate these effects, but each intervention should be assessed for its impact on end-of-life behaviour.

5. Applications in Sustainable Electronics

5.1 Sensors and Wearable Electronics

RC-based sensors can detect pressure, strain, humidity, temperature, chemical species, or biological signals when combined with suitable active materials. Mechanical deformation may change conductive-network contacts and produce a resistance response; humidity can alter water adsorption and ionic or dielectric behaviour; and selective coatings can interact with target molecules. The flexibility and potential biocompatibility of cellulose make it relevant to wearable patches, smart textiles, and disposable sensing platforms. For practical use, however, sensitivity alone is insufficient. Response time, selectivity, hysteresis, drift, repeatability, skin compatibility, and stability under sweat and repeated bending must also be reported [7].

5.2 Actuators and Flexible Circuits

Actuation can be achieved when RC composites respond to humidity, electrical stimulation, heat, or ion migration. Differences in swelling or contraction across layered structures can produce bending and motion, making cellulose-based architectures interesting for soft robotics and responsive interfaces. In flexible circuits, RC may act as a substrate or carrier for printed conductive tracks and components. The main design challenge is maintaining electrical continuity while the substrate bends, stretches, or absorbs moisture. Encapsulation and patterning methods must be compatible with low-cost manufacturing and should avoid making the complete device difficult to recycle [8].

5.3 Energy Harvesting and Storage

Cellulose structures can support energy-harvesting devices by acting as flexible scaffolds, porous separators, dielectric layers, or components of triboelectric and piezoelectric systems. In such devices, mechanical motion is converted into an electrical output through contact electrification, polarization, or deformation of an active composite. Cellulose itself should not automatically be described as a high-performance piezoelectric material; device output depends on the architecture and the active phase used. For energy storage, RC membranes and porous frameworks can serve as separators or hosts for electrodes and electrolytes in batteries and supercapacitors. Their porosity and wettability can assist ion transport, but electrochemical stability, electrolyte compatibility, dimensional integrity, and cycling durability must be demonstrated [9].

5.4 Electromagnetic-Interference Shielding

Modern electronics require protection from electromagnetic interference (EMI). RC composites containing conductive carbon, metallic networks, or other functional fillers can attenuate electromagnetic waves through reflection, absorption, and internal multiple scattering. Cellulose offers a lightweight framework that can reduce reliance on bulk metal components in selected applications. Shielding performance must be considered alongside thickness, density, flexibility,

thermal stability, and environmental impact. A high shielding value alone does not establish sustainability if the composite contains persistent additives or requires energy-intensive processing [10]. Figure 2 shows the different applications for RC in electronics.

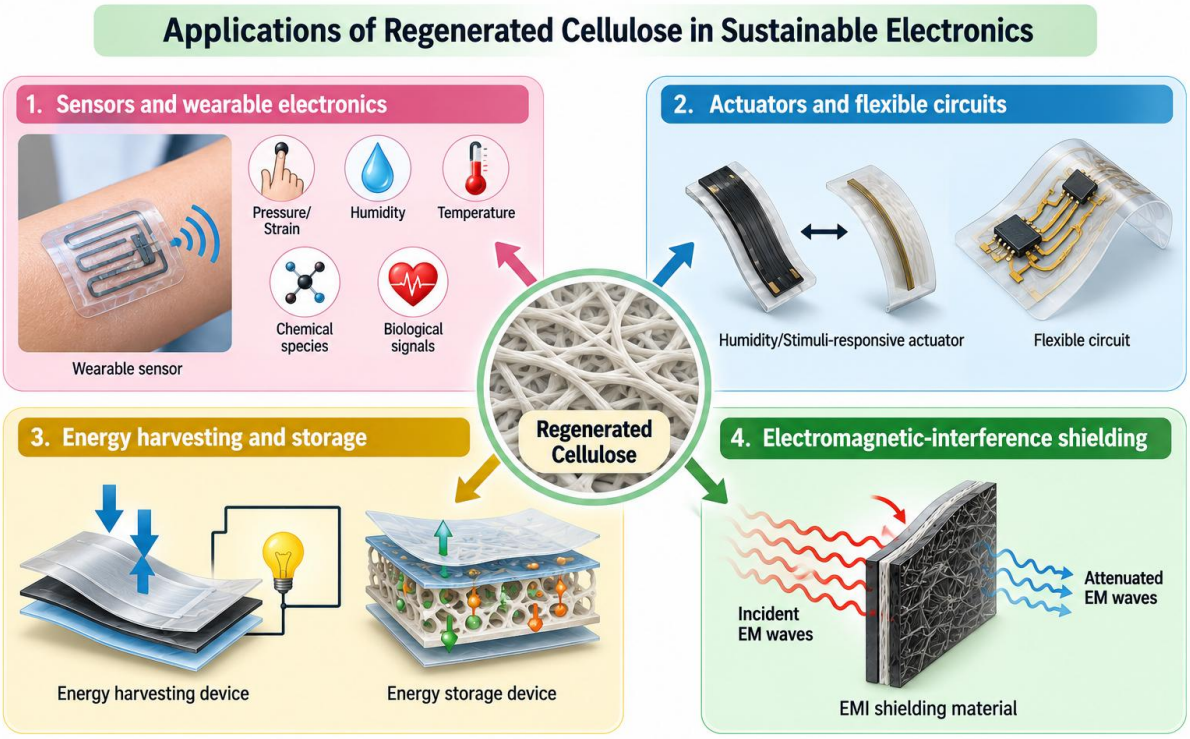


Figure 2: Different applications for RC in electronics

6. Sustainability, Limitations, and Research Needs

The sustainability of RC electronics depends on the whole device, not only the cellulose substrate. Renewable feedstock and potential biodegradability are valuable attributes, but they do not guarantee that a finished electronic product will biodegrade safely. Conductive metals, carbon nanomaterials, binders, crosslinkers, encapsulants, and electrolytes may remain in the environment or complicate recovery. End-of-life testing should therefore examine the complete composite under realistic conditions and assess both cellulose degradation and the fate of functional additives.

Several barriers require attention. First, moisture sensitivity can compromise dimensions and device calibration. Second, conductive and mechanical performance may compete: more filler can improve conductivity but reduce flexibility and transparency. Third, laboratory-scale dissolution and regeneration methods may use costly or hazardous solvents and may not translate directly to continuous manufacturing. Fourth, long-term reliability under repeated bending, temperature cycling, sweat, ultraviolet exposure, and electrical loading remains essential for real-world adoption. Finally, comparisons between studies are difficult when test conditions, sample thicknesses, humidity, device geometries, and reporting standards differ. Figure 3 shows the challenges in RC electronics.

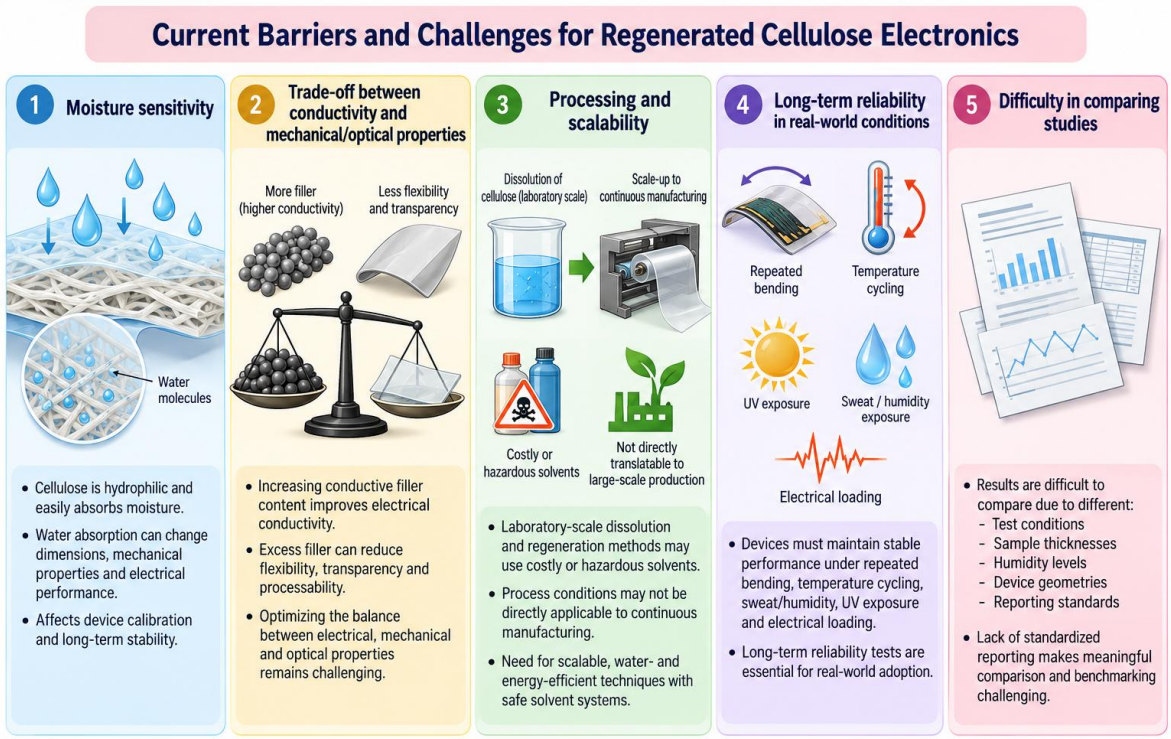


Figure 3: Challenges in RC electronics

Future research should prioritize safer solvent systems, closed-loop solvent recovery, water- and energy-efficient processing, and scalable coating, printing, and fibre-forming techniques. Standardized reporting should include mechanical and electrical performance before and after environmental ageing, material mass balance, solvent recovery, and end-of-life assessment. Life-cycle assessment and techno-economic analysis should compare complete devices with realistic commercial alternatives. Design for disassembly, recovery of valuable conductive components, and selective degradation of the cellulose phase could help reconcile device durability during use with manageable end-of-life treatment.

Conclusions

Regenerated cellulose is a versatile platform for more sustainable electronic devices because it combines renewable origin, adaptable morphology, useful mechanical properties, and compatibility with functional composites. Its potential spans sensors, actuators, flexible circuits, energy harvesting and storage, and EMI shielding. Performance is determined by the interplay of molecular structure, dissolution and regeneration, interfacial design, and the distribution of functional phases. Nevertheless, sustainability should be demonstrated rather than assumed: solvent management, moisture resistance, device lifetime, additive toxicity, recyclability, and full-device degradation all require careful evaluation. Progress will depend on integrated materials design in which electronic performance, manufacturability, and environmental responsibility are optimized together.

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FUNDAMENTAL PROPERTIES AND SYNTHESIS OF SILVER SULPHIDE THIN FILMS

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1. Introduction

Semiconductor thin films have become important functional materials in modern materials science because their structural, optical, electrical, and chemical properties can be tailored through the selection of composition, deposition technique, and processing conditions. They are widely investigated for solar cells, photodetectors, sensors, optical coatings, microelectronic components, and energy-conversion systems. Within this field, metal chalcogenides have received considerable attention because their electronic structures and optical properties can be adjusted through chemical composition, crystal structure, and defect engineering.

Silver sulphide, with the chemical formula Ag_2S, is a significant member of the metal chalcogenide family. It is a binary compound composed of silver and sulphur and is commonly known in its naturally occurring mineral form as acanthite. At ordinary temperatures, Ag_2S generally adopts a monoclinic crystal structure. Its distinctive phase-transition behaviour and silver-ion mobility at elevated temperatures make it interesting for both semiconductor physics and solid-state ionics. The optical band gap of low-temperature monoclinic Ag_2S is commonly reported in the range of 0.9 to 1.1 eV, although the measured value depends on the sample structure, preparation conditions, and analytical method. This relatively narrow band gap makes Ag_2S attractive for near-infrared optoelectronics and photovoltaic research. Its potential advantages include strong optical absorption, the possibility of solution-based fabrication, and useful electronic and mechanical properties. Recent reviews have examined Ag_2S-based thin-film solar cells and flexible thermoelectric devices, highlighting the importance of crystallinity, interfaces, and charge transport in determining device performance [1,2].

The properties of Ag_2S are highly dependent on its preparation method. Variations in precursor concentration, solution pH, deposition temperature, deposition duration, sulphur availability, and post-deposition treatment can modify the phase composition, crystallite size, surface morphology, and defect population. Consequently, systematic control of synthesis conditions is essential for obtaining films with reproducible properties.

Chemical bath deposition is particularly attractive for Ag_2S thin films because it can be performed using relatively simple laboratory equipment and does not require a high-vacuum

environment. Other methods, including SILAR, electrodeposition, spray pyrolysis, and thermal sulphurization, offer alternative routes for controlling film growth and microstructure.

The present chapter provides a comprehensive discussion of the synthesis, structure, properties, and applications of Ag_2S thin films, with particular emphasis on solution-based deposition and the relationships between material characteristics and functional performance.

2. Fundamental Properties of Silver Sulphide

Silver sulphide is a binary inorganic compound with the formula Ag_2S. Its ideal stoichiometric composition contains two silver atoms for every sulphur atom. The corresponding theoretical mass composition is 87.1% silver and 12.9% sulphur. The material belongs to the metal chalcogenide family and exhibits distinct structural and transport characteristics depending on temperature. Under ordinary conditions, the monoclinic phase is the most relevant form for semiconductor thin-film applications. Important properties of Ag_2S include a narrow optical band gap, generally reported 0.9–1.1 eV for monoclinic material, strong absorption extending into the near-infrared region, temperature-dependent structural and transport behavior, and potential compatibility with low-temperature solution-processing methods. It has appplications in optoelectronics, photovoltaics, sensing, thermoelectricity, and resistive switching.

Although Ag_2S is often investigated as a comparatively less hazardous alternative to some cadmium- or lead-containing semiconductors, silver-containing materials still require appropriate environmental and waste-management practices. One of the most distinctive features of silver sulphide is its polymorphism. Different crystal structures become stable over different temperature ranges.

Table 1: Principal polymorphic forms of silver sulphide

Phase	Common Name	Structure	General Structure
α-Ag_2S	Acanthite	Monoclinic	Stable at ordinary temperatures; semiconducting
β-Ag_2S	Argentite	Body-centred cubic arrangement	High-temperature superionic phase
γ-Ag_2S	High-temperature cubic phase	Face-centred cubic arrangement	Stable at still higher temperatures

The α-to-β transition occurs near 450 K, with the precise transition temperature depending on experimental conditions and material characteristics. The β phase exhibits substantially enhanced silver-ion mobility and superionic behaviour. A further structural transformation occurs at higher temperatures, around 860 K under equilibrium conditions [3]. These transitions are important because the crystal structure determines the arrangement of silver and sulphur atoms, the mobility of silver ions, and the electronic and ionic transport characteristics. For thin-film applications, the phase present at room temperature must be established experimentally. A

diffraction pattern that appears consistent with monoclinic Ag_2S should be compared with an appropriate reference pattern, considering possible overlapping peaks, secondary phases, and substrate contributions.

The electronic properties of Ag_2S arise from interactions between silver-derived electronic states and sulphur-derived states. The resulting band structure determines the absorption threshold, charge-carrier behaviour, and response to illumination. The relatively narrow band gap enables absorption of photons with lower energies than those typically absorbed by wide-band-gap semiconductors. This characteristic is valuable for near-infrared photodetection and photovoltaic absorber research. However, a narrow band gap alone does not establish device suitability. Carrier mobility, carrier lifetime, defect density, interfacial band alignment, and resistance to degradation must also be considered.

3. Synthesis of Ag_2S Thin Films

The synthesis method determines the thickness, crystallinity, composition, morphology, adhesion, and defect concentration of Ag_2S films. Various physical and chemical approaches have been reported.

3.1 Chemical Bath Deposition

Chemical bath deposition is a solution-based technique in which a substrate is immersed in a reaction bath containing a silver precursor, a sulphur source, and, where necessary, suitable complexing or stabilizing agents. The method is attractive because of its relatively low equipment cost, simple operation, potential for large-area deposition, and compatibility with glass and other suitable substrates.

Silver nitrate ($AgNO_3$) is commonly used as a silver precursor, while thiourea and sodium thiosulphate are among the sulphur-containing reagents investigated for Ag_2S formation. The general stages of chemical bath deposition are preparation of the precursor solution, regulation of silver-ion availability and sulphur-species formation, establishment of suitable supersaturation conditions, nucleation of Ag_2S on the substrate, growth and coalescence of nuclei, formation of a continuous film, washing, drying, and optional post-deposition treatment.

The deposition process must be optimized to favour film growth over uncontrolled precipitation in the bulk solution. The chemistry of silver is particularly important because silver ions can react rapidly with sulphide-containing species to form poorly soluble silver sulphide [4-5].

3.1.1 Role of the Silver Precursor

Silver nitrate is widely used because it is readily soluble in water and supplies Ag^+ ions. The silver-ion concentration affects the rate of nucleation, the availability of silver for film growth, and the possibility of forming unwanted precipitates. Excessively high silver-ion concentrations may lead to rapid precipitation, rough surfaces, or poor thickness uniformity. Conversely, an insufficient concentration may result in slow growth or incomplete substrate coverage.

3.1.2 Role of the Sulphur Precursor

Thiourea and sodium thiosulphate can provide sulphur for Ag_2S formation through different reaction pathways. Thiourea can generate reactive sulphur-containing species under appropriate chemical and thermal conditions. Sodium thiosulphate can participate in solution reactions that produce silver-containing intermediates and subsequently Ag_2S. The choice of sulphur source influences reaction kinetics, precursor stability, nucleation, and film morphology. The actual mechanism should be interpreted in relation to the selected bath composition rather than assuming that all sulphur precursors behave identically.

3.1.3 Influence of Complexing Agents

Complexing agents can regulate the free silver-ion concentration and modify the rate of precipitation. Their suitability depends on their binding strength, chemical stability, and behaviour under the selected reaction conditions. A complexing agent that binds silver too strongly may inhibit deposition, whereas insufficient complexation may permit rapid precipitation. The optimum concentration must therefore be established experimentally.

3.1.4 Influence of Deposition Temperature and Time

Temperature affects the reaction rate, diffusion, nucleation, and growth of Ag_2S. Deposition time influences thickness, coverage, and the evolution of surface morphology. At short deposition times, isolated nuclei or incomplete coverage may be observed. As deposition proceeds, nuclei may grow and merge to form a more continuous film. Excessive deposition time, however, may promote roughness, particle aggregation, or the formation of loosely attached deposits.

3.2 Successive Ionic Layer Adsorption and Reaction

The successive ionic layer adsorption and reaction technique, commonly known as SILAR, involves alternate exposure of the substrate to solutions containing the constituent ions, with rinsing steps between exposures. For Ag_2S deposition, the substrate is exposed to a silver-containing solution and subsequently to a sulphur-containing solution. Surface reactions during successive cycles lead to the formation and growth of the compound. The film thickness can be adjusted by changing the number of deposition cycles, solution concentrations, immersion durations, and rinsing conditions. SILAR is suitable for substrates that are compatible with aqueous processing and offers a straightforward approach to controlling the amount of deposited material. The main limitations include possible accumulation of loosely attached particles, nonuniform growth, and sensitivity to the chemistry of each adsorption and reaction step.

3.3 Electrodeposition

Electrodeposition uses electrochemical reactions to form a solid layer on an electrically conductive substrate. The deposited material depends on the electrolyte composition, applied potential, current density, temperature, and deposition time. This method can offer control over

deposition rate and film morphology. However, producing phase-pure Ag_2S requires appropriate control of the electrochemical conditions and the relative incorporation of silver and sulphur.

3.4 Spray Pyrolysis

In spray pyrolysis, a precursor solution is atomized and directed towards a heated substrate. Solvent evaporation and subsequent chemical reactions generate the film. The technique can be adapted for relatively large-area coatings, but the quality of Ag_2S films depends on substrate temperature, droplet size, solution composition, spray rate, and the chemical stability of the precursors.

3.5 Thermal Sulphurization

Thermal sulphurization generally involves exposing a silver-containing precursor layer to a sulphur-containing environment at a controlled temperature. Chemical reactions convert the precursor into Ag_2S. The method offers an alternative route to controlling film thickness and morphology through the initial silver layer and sulphurization conditions. The resulting phase and microstructure depend on temperature, reaction time, sulphur availability, and diffusion through the developing film.

3.6 Solution Processing and Coating Methods

Colloidal Ag_2S nanoparticles can be synthesized in solution and subsequently deposited by techniques such as spin coating. Multiple coating cycles can be used to increase film thickness and improve coverage. A recent study demonstrated solution synthesis of α-Ag_2S nanoparticles and the fabrication of multilayer thin films with controlled thickness and surface coverage. The resulting films also exhibited resistive switching behaviour, illustrating the connection between solution processing and emerging electronic applications [6].

3.7 Comparison of Synthesis Methods

Table 2: Comparison of selected Ag_2S deposition techniques

Technique	Principal Advantage	Important Consideration
Chemical bath deposition	Simple, low-cost solution processing	Control of precipitation and stoichiometry
SILAR	Thickness adjustment through repeated cycles	Uniformity and particle adhesion
Electrodeposition	Electrochemical control of growth	Conductive substrate and potential optimization
Spray pyrolysis	Potential for large-area coatings	Temperature and droplet control
Thermal sulphurization	Conversion of a precursor layer into Ag_2S	Sulphur diffusion and phase control
Spin coating of colloidal Ag_2S	Convenient multilayer fabrication	Film density, drying, and interlayer quality

The most appropriate technique depends on the required thickness, substrate, device architecture, processing cost, and desired electronic properties.

4. Reaction Chemistry and Growth Mechanism

4.1 Formation of Silver Sulphide

The formation of Ag_2S requires the reaction of silver-containing species with reactive sulphur species. A simplified net ionic equation is $2Ag^+ + S^{2-} \rightarrow Ag_2S(s)$. This equation represents the overall stoichiometric formation of silver sulphide. It does not necessarily describe the elementary steps occurring in a chemical bath, where the free sulphide-ion concentration may be very low and intermediate species may participate. For a thiosulphate-based route, silver thiosulphate may form as an intermediate before decomposing or reacting to yield Ag_2S. A simplified representation of the intermediate formation is: $2Ag^+ + S_2O_3^{2-} \rightarrow Ag_2S_2O_{3\,(s)}$. Subsequent reactions can produce silver sulphide under suitable conditions. The detailed pathway depends on the solution composition and experimental conditions.

4.2 Nucleation

Nucleation is the initial formation of stable Ag_2S clusters. In a deposition bath, nucleation may occur on the substrate surface, in the bulk solution, or at both locations. Heterogeneous nucleation on the substrate is desirable for forming an adherent coating. Homogeneous nucleation in the solution may generate suspended particles that subsequently deposit loosely on the film or settle at the bottom of the reaction vessel. The relative importance of these pathways depends on supersaturation, substrate surface energy, precursor concentration, temperature, and reaction rate [7].

4.3 Crystal Growth

After nucleation, additional silver- and sulphur-containing species attach to existing nuclei. Growth proceeds through surface reactions, diffusion, and incorporation into the crystal lattice. The rate of crystal growth influences crystallite size, film compactness, and surface roughness. A balance between nucleation and growth is generally required to obtain a uniform film.

4.4 Coalescence and Film Formation

As nuclei grow, neighbouring islands may merge to form a continuous layer. Subsequent deposition increases thickness and can modify the surface morphology. The final microstructure depends on deposition duration, solution stability, substrate preparation, and the relative rates of nucleation and growth. The mechanism should be established from experimental evidence rather than inferred solely from a final SEM image.

4.5 Influence of Deposition Parameters

The influence of each parameter should be evaluated through controlled experiments, with one or more variables changed systematically.

Table 3: Important parameters affecting Ag_2S film growth

Parameter	Possible Effect on Film Formation
Silver-ion concentration	Changes nucleation rate and availability of silver
Sulphur precursor concentration	Influences sulphur supply and precipitation kinetics
Temperature	Alters reaction rate, diffusion, and crystallite growth
Deposition time	Affects thickness, coverage, and surface morphology
Complexing-agent concentration	Modifies silver-ion availability
Bath composition and pH	Influences precursor speciation and reaction pathways
Substrate cleanliness	Affects nucleation density and adhesion
Post-deposition annealing	May modify crystallinity, defects, and grain structure

5. Applications and Future Opportunities of Ag_2S Thin Films

Silver sulphide thin films have attracted considerable research interest because of their narrow band gap of 0.9–1.1 eV, strong absorption in the near-infrared region, and temperature-dependent electrical and ionic transport properties. These characteristics make Ag_2S a promising material for photovoltaic devices, photodetectors, sensors, thermoelectric systems, and other optoelectronic applications.

Photovoltaic and solar-energy applications: Ag_2S is a potential absorber material for thin-film solar cells because its narrow band gap enables the utilization of a substantial portion of the solar spectrum. Solution-based deposition methods, such as chemical bath deposition (CBD), offer opportunities for fabricating thin films at relatively low temperatures and low cost. Further improvements in film uniformity, interface quality, carrier transport, and device stability are required to achieve reproducible and efficient photovoltaic performance.

Photodetectors and optoelectronic devices: The near-infrared absorption characteristics of Ag_2S make it attractive for photodetection, optical sensing, and light-responsive electronic devices. Ag_2S-based heterostructures and composite films may improve charge separation and photoresponse. Future research should focus on optimizing film thickness, controlling defects, and engineering interfaces to enhance sensitivity, response speed, and long-term stability.

Thermoelectric and sensing applications: Ag_2S exhibits temperature-dependent transport properties, making it relevant to thermoelectric research and temperature-sensitive devices. The development of Ag_2S-based composites and flexible films may provide opportunities for low-temperature energy harvesting and wearable electronics. However, its phase transitions and changes in ionic conductivity must be carefully considered when designing devices for practical operating conditions. Ag_2S is also being investigated for chemical and environmental sensing, where changes in its electrical or optical response can be used to detect target species.

Future Opportunities

Future research on Ag_2S thin films should prioritize precise control of stoichiometry, crystal structure, crystallite size, defect concentration, and surface morphology. Optimizing chemical bath deposition parameters—including precursor concentration, pH, complexing agent, bath temperature, and deposition time—could improve film continuity and reproducibility. The incorporation of suitable dopants, formation of semiconductor heterojunctions, and fabrication of Ag_2S-based nanocomposites offer additional approaches to tailoring charge transport and optical absorption. Advanced characterization techniques, including time-resolved spectroscopy, impedance analysis, and temperature-dependent structural measurements, could provide deeper insight into charge-carrier dynamics and phase stability. Furthermore, future studies should include standardized device testing, long-term operational stability, scalable fabrication, and comparisons with established absorber and sensor materials. Overall, Ag_2S thin films offer promising opportunities for next-generation optoelectronic and energy-conversion technologies, provided that their structural stability, device performance, and manufacturing reproducibility are systematically improved.

6. Limitations of Ag_2S Thin Films

Despite their promising optical and electrical properties, silver sulphide thin films face several limitations that restrict their practical applications. The properties of Ag_2S are strongly influenced by deposition conditions, stoichiometric variations, structural defects, and surface morphology, making it difficult to obtain films with consistent quality and reproducible performance. Nonuniform film thickness, poor adhesion, surface porosity, and the formation of secondary phases may adversely affect charge transport and device efficiency. Although Ag_2S exhibits a narrow band gap of 0.9–1.1 eV, defects and grain boundaries can promote carrier recombination and increase electrical losses. Furthermore, its temperature-dependent phase transitions can significantly alter its transport behaviour, particularly under elevated-temperature operating conditions. In photovoltaic and photoelectrochemical devices, challenges associated with interfacial charge transfer, contact resistance, operational stability, and reproducibility must be addressed. The use of silver-containing precursors may also increase material costs compared with some alternative semiconductor systems. In addition, variations in deposition methods and characterization procedures can complicate comparisons between reported results. Therefore, further research is required to optimize deposition parameters, control composition and defects, improve film stability, and establish scalable fabrication methods for reliable Ag_2S thin-film devices.

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BRIDGING DISCOVERY AND DEPLOYMENT: QUANTIFYING TRENDS, TECHNOLOGY READINESS AND REAL-WORLD SOLUTIONS IN SCIENCE AND ENGINEERING RESEARCH

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Abstract
Science and engineering research has accelerated markedly the translation of discoveries into scalable real-world solutions remains uneven. This perspective paper examines progress across six high-impact domains—artificial intelligence for scientific discovery, advanced energy storage, quantum technologies, CRISPR-enabled gene editing and synthetic biology, advanced semiconductors, and climate-adaptation engineering—by linking measurable research trends to technology readiness levels (TRLs) and concrete deployments (commercial products, policy adoption, and scaled pilots). Drawing on bibliometric data, funding reports, patent analyses, and verified project outcomes. The analysis identifies enabling factors (agentic AI systems, public–private partnerships, and targeted industrial policy) and persistent barriers (manufacturing scale-up, regulatory pathways, and equity of access). Findings offer actionable insights for researchers, funders, and policymakers seeking to accelerate the conversion of scientific advances into societal benefit.

Keywords: Scientific Research, Technology Translation, TRLs, Scalable Solutions, Commercialization, Industrial Policy, High-Impact Domains.

1. Introduction

Recent years have witnessed an extraordinary expansion of scientific output and engineering capability. Publication volumes in key fields have risen sharply, public and private funding have surged in strategic areas, and citation networks have intensified around breakthrough methods. At the same time, society faces urgent demands for solutions in energy security, health, climate resilience, and advanced computing. The central challenge is no longer solely the generation of new knowledge but the speed and reliability with which that knowledge reaches commercial products, policy frameworks, or large-scale pilots.

This paper addresses that challenge by posing and examining six sharply focused research questions that explicitly connect measurable research trends with technology readiness and documented real-world outcomes:

i. How have shifts in publication volume, citation impact, and funding for artificial intelligence methods in scientific discovery correlated with the TRLs (Technology

Readiness Levels) and commercial deployment of AI-driven tools in materials science, drug discovery, and climate modeling?

ii. To what extent has growth in research output and citation impact in next-generation battery and energy-storage materials translated into higher TRLs and measurable market penetration of commercial products or grid-scale pilots?

iii. What is the relationship between rising research funding, publication trends, and citation networks in quantum computing and sensing and the progression from laboratory demonstrations to early commercial products or government-backed pilots?

iv. How have changes in publication volume, interdisciplinary citation patterns, and targeted funding for CRISPR-based and synthetic-biology platforms influenced the speed and scale of translation into approved therapeutics, agricultural products, and industrial bio-manufacturing?

v. In what ways have increases in research activity and citation impact in advanced semiconductor materials and chip-design methodologies corresponded with technology readiness advances and commercial or policy-driven deployment of next-generation computing hardware?

vi. How has the trajectory of research funding, publication growth, and citation influence in climate-adaptation and nature-based engineering solutions mapped onto TRLs and documented adoption in national policy frameworks or large-scale infrastructure pilots?

By synthesizing evidence across these questions, the paper contributes a structured assessment of where science and engineering progress has most successfully crossed the "valley of death" between discovery and deployment.

2. Methodology

This work is a structured perspective and evidence synthesis rather than a primary empirical study. We conducted a multi-source review covering 2018–2026. Primary data sources included:

i. Bibliometric indicators from OpenAlex, Scopus, and Web of Science (publication counts, citation distributions, and field-normalized impact).

ii. Funding data from public agencies (NSF, DOE, EU Horizon, national programmes) and private investment trackers (McKinsey Technology Trends Outlook, venture reports).

iii. Patent statistics from WIPO and national offices, focusing on generative AI, solid-state batteries, quantum hardware, and gene-editing platforms.

iv. Technology readiness assessments drawn from agency reports, company disclosures, and independent analyses (TRL 1–9 scale).

v. Documented deployments verified through peer-reviewed case studies, regulatory approvals, company press releases, and independent project trackers (e.g., battery storage project databases, CRISPR therapy sales reports, quantum cloud access announcements).

Trends were prioritized if they demonstrated both strong research metrics and at least two independent real-world deployments at TRL 6 or higher. Quantitative claims are anchored to publicly reported figures; qualitative assessments of barriers and enablers draw on convergent evidence from multiple sources.

3. Key Trends, Indicators, and Real-World Translations

3.1 Artificial Intelligence for Scientific Discovery

Publication volume of AI-augmented scientific papers rose sharply, with AI accounting for 5.8–8.8 % of output in several natural-science fields by 2025. Generative-AI patent families more than doubled between 2023 and 2025. Agentic systems (e.g., multi-agent hypothesis generation and automated experimental design) have reached TRL 7–8 in materials and biological discovery. Documented outcomes include experimentally validated drug-repurposing candidates, rapid screening of millions of crystal structures yielding confirmed superconductors, and an AI-assisted original drug approved after a markedly shortened development timeline.

3.2 Next-Generation Energy Storage

Research output and citation impact in solid-state, sodium-ion, and advanced lithium systems grew rapidly, supported by substantial public and private funding. Semi-solid and sodium-ion solutions have reached TRL 8–9; all-solid-state systems sit at TRL 6–7. Real-world deployments include multi-GWh contracted sodium-ion grid storage already in commercial operation, full-capacity solid-state pilot lines supplying energy-storage and mobility applications, and rapid conversion of existing manufacturing lines to stationary-storage production.

3.3 Quantum Computing and Sensing

Funding rose fivefold in a single recent year, while publication and citation activity continued upward. Cloud-accessible systems and early quantum-as-a-service offerings operate at TRL 5–7. Concrete deployments include utility-hosted commercial quantum computers offering external access, industrial QaaS platforms, and hybrid quantum–classical installations at national laboratories.

3.4 CRISPR-Based Gene Editing and Synthetic Biology

Publication and funding growth, together with intensive interdisciplinary citation networks, supported the first approved CRISPR therapy (Casgevy/exa-cel). The therapy has reached TRL 9, with regulatory expansion to younger paediatric populations and commercial treatment centres operating in multiple countries. Precision-fermentation platforms for animal-free proteins have similarly advanced to commercial retail products and industrial-scale manufacturing plants.

3.5 Advanced Semiconductors and Chip Design

Although detailed quantitative deployment data remain more fragmented, research activity and citation impact have tracked closely with industrial and policy-driven capacity expansion (CHIPS-related investments, advanced packaging, and AI-specific accelerators). Leading

solutions sit at high TRL for commercial production, with policy frameworks explicitly linking research advances to manufacturing deployment.

3.6 Climate-Adaptation and Nature-Based Engineering

Funding and publication trends in climate-resilient materials, nature-based solutions, and flexible grid resources have mapped onto rising TRLs and policy adoption. Everything-to-grid architectures and distributed energy resources have demonstrated measurable grid services (e.g., peak-shaving contributions exceeding conventional peaker plants in documented events). Direct lithium extraction, a critical materials technology for energy transition, has moved from pilot to commercial plants in multiple jurisdictions.

4. Discussion

Across the six domains, three patterns emerge. First, fields that combine rapid algorithmic or methodological advance with strong industrial demand (AI for discovery, energy storage, gene editing) have achieved the fastest translation. Second, public–private partnerships and targeted industrial policy have been decisive enablers of scale-up. Third, persistent gaps remain in manufacturing yield, long-term reliability data, regulatory harmonization, and equitable access—particularly for advanced therapeutics and capital-intensive hardware.

The analysis supports a cautious optimism: several research trajectories that were laboratory curiosities in 2018 now deliver measurable societal and economic outcomes. Continued progress will depend on maintaining investment in both fundamental science and the engineering, regulatory, and market infrastructures that convert discovery into durable solutions.

Conclusion

Science and engineering research in recent times have produced not only an expansion of knowledge but a demonstrable narrowing of the gap between discovery and deployment in several strategically important domains. By systematically linking publication, funding, citation, and patent indicators to technology readiness levels and verified real-world outcomes, this paper provides a framework for assessing translational progress. The evidence indicates that targeted investment, interdisciplinary collaboration, and deliberate translation mechanisms can convert research excellence into tangible solutions. Future work should extend this mapping to additional domains and develop more granular metrics of societal impact beyond commercial deployment alone.

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