ISSN (ONLINE) 2583-2506

http://publications.rayatbahrauniversity.edu.in

RBIJMR-Rayat Bahra International Journal of Multidisciplinary Research, Vol. 05, Issue 02,Dec2025

AI and IoT in Sustainable Nanotechnology: Opportunities and Case Studies

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Abstract: *Artificial Intelligence (AI) and the Internet of Things (IoT) are revolutionizing sustainable nanotechnology by enhancing material design, improving process efficiency, and enabling real-time monitoring across a range of applications. This chapter explores how AI and IoT are integrated into the development, deployment, and lifecycle management of nonmaterial's to promote environmental and economic sustainability. Through a blend of theoretical insights and practical case studies, the chapter highlights current progress, challenges, and emerging opportunities in this interdisciplinary domain. This book chapter will serve as a guide to the professionals, academicians, researchers, and students for further investigations and developments in the field.*

Keywords: Nanotechnology, Sustainable, Artificial Intelligence, Internet of Things, Technology, Nanomaterials, Intelligent Systems, Optimization, Environment

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1. Introduction

Sustainable nanotechnology focuses on minimizing the environmental and health impacts of nanomaterials throughout their lifecycle. The convergence of AI and IoT technologies with nanotechnology provides new avenues for making nonmaterial synthesis greener, usage more efficient, and disposal safer. AI enables predictive modelling and design optimization, while IoT facilitates real-time data collection and environmental monitoring, together contributing to sustainable practices [1]. Beyond their individual capabilities, the synergy of AI and IoT fosters the creation of intelligent, autonomous systems that can adapt dynamically to environmental inputs. These technologies also enable closed-loop systems that align with circular economy principles, making nanotechnology not only advanced but also ethically and environmentally responsible.

2. AI in Sustainable Nanotechnology

AI is transforming sustainable nanotechnology by enabling faster, safer, and more environmentally responsible design and production of nanomaterials. When artificial intelligence is integrated with nanotechnology**,** it enhances design, synthesis, and analysis of nonmaterial’s with a focus on sustainability**,** reducing environmental impact, energy usage, and material waste. Different applications of AI in sustainable nanotechnology are as given below:

2.1 Nanomaterials Discovery and Design

AI techniques like machine learning (ML) and deep learning (DL) accelerate the discovery of novel nanomaterials by predicting their properties and behaviors based on structural data. Algorithms can:

- Screen thousands of potential materials for specific functions.
- Optimize synthesis conditions.
- Predict toxicity and environmental impact.

Case Study 1: The Materials Project and Citrine Informatics have used ML to predict the thermodynamic stability of nanomaterials, reducing trial-and-error experiments by over 60% [2].

Case Study 2: A collaborative project between the National Institute of Standards and Technology (NIST) and IBM Research employed generative adversarial networks (GANs) to design high-performance polymer nanocomposites [3]. The system identified combinations with optimal mechanical strength and thermal stability, reducing development time by 45%.

2.1.1 Advantages and Disadvantages

Advantages

- **Accelerated Discovery :**

  AI can process vast datasets to identify promising nanomaterials , significantly reducing the time required for discovery.

- **High-Throughput Screening:**

Algorithms evaluate thousands of material candidates for target properties, such as conductivity or biocompatibility, more efficiently than traditional methods.

Case Study: Citrine Informatics uses AI for high-throughput screening of polymer nanocomposites with optimized mechanical properties.

- **Cost and Resource Efficiency**

By minimizing the number of required lab experiments, AI reduces waste, labor, and material costs during early-stage development. Kim et al. (2020) reported that AI-guided synthesis cut energy use in nanoparticle development by 30% [4].

- **Design of Custom Materials**

Generative models like GANs and reinforcement learning approaches help design novel nanostructures tailored to specific functions (e.g., drug delivery, catalysis).

- **Toxicity and Environmental Impact Prediction**

AI tools can predict environmental behaviour and potential toxicity of nonmaterial's, supporting safe-by-design principles. Maynard has reported it in one of his findings [5].

Disadvantages

- **Data Limitations and Bias**

High-quality, labelled datasets for nonmaterial's are often incomplete or domain-specific, leading to model inaccuracies and overfitting.

- **Black-Box Nature of AI Models**

Many AI models, especially deep learning ones, lack interpretability, making it difficult to validate decisions or understand underlying mechanisms.

- **Generalization Challenges**

Models trained on specific nanomaterials may not generalize well to other systems due to high variability in nanoscale behaviors.

- **Dependence on Domain Expertise**

AI systems still require expert oversight for data curation, model selection, and results interpretation, which can be resource-intensive.

- **Ethical and Regulatory Concerns**

The integration of AI in nanodesign raises regulatory questions regarding data integrity, safety validation, and accountability in automated systems.

2.2 Process Optimization

AI models are used to improve green synthesis techniques by:

- Adjusting parameters like temperature, pH, and precursor concentration.
- Reducing energy and solvent use.
- Enhancing yield and quality of nanoparticles.

Case Study 1: AI-optimized sol-gel methods for ZnO nanoparticles have achieved a 30%

reduction in energy consumption compared to conventional approaches.

Case Study 2: Researchers at the University of Tokyo developed a neural network model to optimize the hydrothermal synthesis of TiO2 nanostructures, improving photo catalytic efficiency while cutting processing costs by 25%.

Case Study 3: Deep Mind's AlphaFold has been used to predict the interaction of protein-nanoparticle complexes, streamlining design processes in nanomedicine.

2.2.1 Advantages and Disadvantages

Advantages

- **Enhanced Efficiency and Yield**

AI algorithms optimize synthesis parameters (e.g., temperature, pressure, concentration) in real time, reducing energy and material waste while improving nanoparticle yield and quality.

- **Precision and Reproducibility**

Machine learning models reduce variability by identifying optimal operating windows, thus improving consistency across batches. Neural networks applied to hydrothermal synthesis of TiO_2 nanostructures enhanced photocatalytic efficiency and reduced production costs [6].

- **Real-Time Monitoring and Control**

IoT devices enable live feedback and adaptive control during nanomaterial production, minimizing process deviations. BASF's IoT-guided production line achieved a 40% reduction in water usage.

- **Resource Optimization and Predictive Maintenance**

Smart factories use IoT analytics to monitor machinery and prevent downtime, improving sustainability through better equipment utilization. Siemens' digital twin system integrates IoT and AI to detect inefficiencies in nanomaterial manufacturing [7].

- **Environmental and Safety Improvements**

IoT-connected nanosensors detect emissions and leaks, allowing for rapid intervention and compliance with environmental regulations. Lee et al. Demonstrated graphene-based nanosensors detecting VOCs in industrial zones [8].

Disadvantages

- **Data Dependency and Quality Issues**

AI models require large, high-quality datasets for training. In nanotechnology, such data may be scarce or unstructured, limiting model accuracy.

- **Complexity and Interpretability**

Advanced AI models (e.g., deep learning, GANs) often operate as black boxes, making it difficult to interpret results or trace decisions.

- **Cyber security and Privacy Risks**

IoT systems are vulnerable to cyber threats, which can compromise data integrity or disrupt critical processes. Schmidt emphasizes the importance of robust cyber security frameworks in emerging technologies [9].

- **High Initial Investment**

The deployment of AI and IoT infrastructure especially at scale can be expensive due to the need for specialized sensors, computing hardware, and skilled personnel.

- **Regulatory and Ethical Constraints**

The lack of standardization and ethical guidelines in AI applications, particularly in safety-critical nano processes, can hinder implementation and public acceptance.

2.3 Risk Assessment and Safety

AI facilitates early-stage risk assessment by modeling the interaction of nanomaterials with biological systems and ecosystems. It helps in developing safe-by-design nanomaterials. Maynard suggests that AI-driven toxicological models can fill data gaps in nanomaterial safety profiles [10].

Case Study: The NanoSolveIT project uses AI to predict the environmental and human toxicity of engineered nanomaterials, helping regulators and industries assess risks [11].

2.3.1 Advantages and Disadvantages

Advantages

- **Faster Risk Profiling**

AI models can rapidly predict toxicity, bioaccumulation, and environmental behavior of nanomaterials based on limited experimental data.

- **Safe-by-Design Nanomaterials**

AI tools support the design of nanomaterials with reduced environmental and health risks by integrating safety metrics into the early development phase.

Case Study: NanoSolveIT employs predictive algorithms to screen materials before production, minimizing the need for animal testing.

- **Reduction in Experimental Burden**

AI enables in silico assessments that reduce dependence on costly and time-consuming laboratory or animal testing.

- **Improved Regulatory Support**

Predictive models assist regulators in assessing the potential hazards of nanomaterials with insufficient empirical data.

- **Integration with Real-Time Monitoring**

When paired with IoT sensors, AI systems provide dynamic safety alerts and predictive maintenance in high-risk environments. The MIT Nanotechnology Lab integrated AI with nanosensors to detect harmful nanoparticles in clean rooms, triggering automated ventilation protocols [12].

Disadvantages

- **Lack of Standardized Datasets**

AI accuracy in risk modeling is limited by the scarcity of comprehensive and validated nanotoxicological data.

- **Overfitting and Poor Generalization**

Models trained on narrow datasets may perform poorly on new nanomaterials or under different environmental conditions.

- **Interpretability Challenges**

Many AI algorithms act as "black boxes," making it difficult to explain or justify predictions in a regulatory or clinical context.

- **Ethical and Legal Concerns**

Using AI for toxicology raises concerns about the ethical replacement of traditional safety testing methods without sufficient validation.

- **Computational Resource Demands**

High-fidelity models, especially those using deep learning, can be computationally intensive and inaccessible to smaller labs or regulatory bodies.

3. IoT in Sustainable Nanotechnology

IoT is a powerful enabler of sustainability in nanotechnology by enhancing visibility, control, and optimization across production and application domains. When combined with **nanotechnology**, IoT systems can monitor, control, and optimize nanoscale processes, contributing to **sustainable development** through efficient resource use, waste reduction, and enhanced safety. Different applications of IoT in sustainable nanotechnology are as given below:

3.1 Environmental Monitoring

IoT devices embedded with nano-enabled sensors provide real-time monitoring of air, water, and soil quality. These sensors detect:

- Nanoparticle release and dispersion.
- Heavy metals and toxic compounds.
- Changes in environmental parameters.

Case Study: A smart IoT system deployed in industrial zones in South Korea utilized graphene-based nanosensors to detect VOCs and nanoparticle emissions, enabling rapid response and mitigation.

3.1.1 Advantages and Disadvantages

Advantages

- **Real-Time Monitoring and Early Detection**

IoT-enabled nanosensors provide continuous data streams, enabling early identification of hazardous nanoparticle emissions or environmental changes.

- **High Sensitivity and Precision**

Nanoscale sensors integrated with IoT devices detect contaminants at parts-per-billion (ppb) or even parts-per-trillion (ppt) levels, enhancing response accuracy.

- **Scalability and Remote Accessibility**

IoT systems can be deployed over large geographical areas, transmitting data remotely via wireless networks. A smart water monitoring system using carbon nanotube sensors provided remote updates on heavy metal levels in agricultural runoff.

- Improved Data Analytics and Predictive Maintenance

Collected data can be analyzed using AI to predict system failures or pollutant surges, allowing proactive environmental protection.

- **Support for Regulatory Compliance and Sustainability**

IoT-based environmental tracking ensures industries remain compliant with environmental regulations, while also supporting corporate sustainability reporting. Ellen MacArthur Foundation highlighted IoT's role in data-driven lifecycle assessment and sustainability documentation [13].

Disadvantages

- **Cybersecurity Vulnerabilities**

IoT networks can be susceptible to hacking, data breaches, or unauthorized access, especially when deployed in critical infrastructure.

- **Data Overload and Storage Complexity**

Continuous monitoring generates massive datasets, requiring robust storage infrastructure and data management strategies.

- **High Initial Costs**

The deployment of nanosensors, network infrastructure, and cloud analytics systems requires substantial initial investment. A European Union-funded smart sensing project reported a 25% budget overrun during its pilot phase due to high sensor calibration costs.

- **Maintenance and Calibration Needs**

Nanosensors, though highly sensitive, can degrade over time and require frequent recalibration to ensure accuracy.

- **Limited Interoperability**

Devices from different manufacturers may not be compatible, hindering the integration of monitoring networks across sectors or regions.

3.2 Smart Manufacturing

IoT-enabled smart factories integrate nanosensors and connected machinery to:

- Monitor and control nanomaterial synthesis in real-time.
- Minimize waste and emissions.
- Enable predictive maintenance to reduce downtime.

Case Study1: BASF implemented an IoT-guided nanomaterial production line that reduced water usage by 40% through real-time feedback loops.

Case Study 2: In Germany, a chemical manufacturer implemented IoT-connected reactors using nanoscale thermocouples to maintain optimal synthesis conditions, reducing product defects by 18%.

Case Study 3: Samsung's IoT-powered cleanroom monitoring systems ensure precise nanoparticle control in semiconductor fabrication.

3.2.1 Advantages and Disadvantages

Advantages

- Real-Time Monitoring and Control

IoT sensors allow continuous real-time monitoring of manufacturing processes at the nanoscale, improving precision and reducing defects. It enables precise control of temperature, pressure, and chemical concentrations which is crucial in nonmaterial synthesis [14].

- **Resource and Energy Efficiency**

IoT devices track energy and raw material usage, enabling optimization and reducing waste, which directly supports sustainability goals It reduces carbon footprint and supports circular manufacturing models [15].

- **Predictive Maintenance and Downtime Reduction**

IoT-enabled systems can predict equipment failures using condition monitoring, minimizing unplanned downtime and production interruptions. It extends machine life and reduces unnecessary part replacements [16].

- **Enhanced Supply Chain Transparency**

IoT improves traceability of nano-products from source to end-user, ensuring environmental compliance and quality. It is crucial in validating sustainable sourcing of nano raw materials and supporting green certification [17].

- **Data-Driven Innovation**

The data collected through IoT networks enables continuous process optimization and smart material development, accelerating innovation in nanotechnology. It supports agile experimentation with sustainable nano-formulations [18].

Disadvantages

- **Cyber security Vulnerabilities**

IoT systems are vulnerable to hacking, data breaches, and malware, which can threaten sensitive nano-production processes and IP. It is a major barrier for adoption in high-value nano manufacturing sectors [19].

- **High Initial Infrastructure Costs**

Deploying IoT in nanotechnology manufacturing requires expensive sensors, networks, and integration platforms. It is cost-intensive for small manufacturers focused on sustainable materials [20].

- **Data Overload and Management Challenges**

IoT networks generate massive volumes of data, which require sophisticated analytics and storage solutions to be useful. Without proper data infrastructure, IoT data becomes a burden rather than a benefit [21].

- **Limited Interoperability**

Incompatible IoT devices and platforms can limit integration across different stages of nano-manufacturing, disrupting sustainability tracking. It leads to inefficient systems that require custom bridging solutions [22].

- **Environmental Impact of IoT Devices**

Though IoT promotes sustainability, the production, power consumption, and disposal of sensors and devices may pose environmental risks if not managed properly. Lifecycle impacts must be considered to align with green nanotechnology goals [23].

3.3 Lifecycle Management and Circular Economy

IoT technologies support lifecycle tracking and recycling of nano-enabled products by:

- Embedding RFID or nano-barcodes.
- Monitoring product condition and wear.
- Enabling reverse logistics for recycling and reuse.

Case Study: Philips uses IoT-embedded sensors in medical devices to collect usage data, enabling recycling programs that extract rare earths and nanomaterials for reuse [24].

3.3.1 Advantages and Disadvantages

- **Enhanced Traceability Across the Product Lifecycle**

  IoT technologies such as RFID tags, nano-barcodes, and embedded sensors enable real-time tracking of nano-enabled products from production to disposal.

- **Support for Closed-Loop Recycling Systems**

IoT sensors monitor the condition, usage patterns, and residual value of nanomaterials in products, supporting decisions about repair, reuse, or recycling.

- **Lifecycle Optimization for Sustainability**

Collected data help optimize design and maintenance schedules, minimizing waste generation and extending product lifespan.

- **Improved Resource Efficiency and Emissions Reduction**

  Real-time IoT feedback enables efficient energy use and minimizes material losses during production and end-of-life stages. A German startup used IoT-linked nano-labels to reduce waste in packaging, cutting plastic use by 30% through intelligent re-routing in supply chains.

- **Facilitates Regulatory Compliance and Transparency**

IoT provides traceable, time-stamped data for environmental reporting and compliance with extended producer responsibility (EPR) regulations.

Disadvantages

- **High Capital and Operational Costs**

Embedding sensors and maintaining real-time tracking infrastructure across global supply chains can be prohibitively expensive. A pilot project integrating nano-RFID for lifecycle tracking in consumer electronics faced scalability issues due to sensor cost and battery limitations.

- **Data Privacy and Ownership Issues**

The vast amount of lifecycle data collected raises questions about who owns the data and how it can be ethically used.

- **Technological Interoperability Challenges**

Incompatibility between IoT devices and software platforms can hinder seamless tracking, especially in multi-stakeholder supply chains.

- **Sensor Degradation and Maintenance Requirements**

Long-term use in varying environmental conditions can affect the accuracy and reliability of embedded nanosensors.

- **E-Waste Generation from Obsolete IoT Devices**

Ironically, the use of IoT devices can contribute to electronic waste if their end-of-life is not managed responsibly.

4. Integrated AI-IoT Platforms in Nanotechnology

Combining AI and IoT creates intelligent systems capable of autonomous decision-making and adaptive responses. Applications include:

- Self-regulating air filtration systems using smart nanofibers.
- AI-driven IoT wearables for environmental sensing.
- Automated water purification systems using nano-catalysts.

Case Study 1: MIT developed an integrated AI-IoT water purification system using TiO_2 nanoparticles and sensor-driven feedback loops, achieving 99.8% contaminant removal efficiency with minimal energy use [25].

Case Study 2: In India, a smart irrigation system integrated with AI and nanosensors enabled precision agriculture, reducing fertilizer usage by 35% and water consumption by 40%.

Case Study 3: Siemens uses digital twins that integrate IoT and AI to simulate and optimize nanomaterial production systems, identifying faults and opportunities for sustainability improvement.

5. Challenges and Limitations of AI in Sustainable Nanotechnology

- **Data Scarcity and Quality Issues**

Nanotechnology involves complex, expensive, and highly specialized experiments, resulting in limited datasets**.** AI models struggle to generalize due to insufficient, noisy, or inconsistent data. For example, in nanoparticle synthesis, variations in input materials can produce unpredictable outcomes that AI cannot accurately model without large datasets.

- **Lack of Interpretability (Black Box Problem)**

Many AI models, especially deep learning, lack transparency. Scientists and regulators may distrust AI-driven decisions about sustainable nanomaterials due to unclear reasoning. It is difficult to validate AI-generated green product recommendations without explain ability.

- **High Computational and Energy Costs**

Training large AI models consumes significant computing power. It may contradict the goals of sustainability if not powered by renewable energy sources. For example, the carbon footprint of training deep neural network can offset the environmental gains of the resulting application.

- **Limited Domain-Specific AI Models**

Generic AI models often perform poorly when applied to nano-specific manufacturing contexts. It requires **domain-expert involvement** to customize models, increasing development time and cost.

- **Ethical and Regulatory Uncertainty**

AI-driven decisions in nanotech (e.g., material toxicity predictions) face ethical scrutiny and lack of clear regulation**.** It slows down adoption and commercialization of AI-enabled sustainable solutions.

6. Challenges and Limitations of IoT In Sustainable Nanotechnology

- **Cyber security Risks**

IoT devices are vulnerable to hacking, especially in sensitive nano-manufacturing processes. Security breaches could leak proprietary data or disrupt critical nano-production.

- Device Reliability and Miniaturization
  Sensors must be highly accurate at nanoscale**,** often in extreme environments (high temp, corrosive). Sensor malfunction or drift reduces reliability of real-time data.
- Data Overload and Management

Massive data streams from IoT networks need efficient filtering, processing, and storage**.** Without edge computing or AI integration, this data is underutilized or creates bottlenecks.

- **High Initial Setup and Maintenance Costs**

IoT integration in nano-manufacturing requires expensive, specialized infrastructure. It is cost-prohibitive for small-scale or early-stage sustainable nanotech ventures.

- **Interoperability and Standardization Gaps**

IoT devices often operate on different protocols or platforms. It limits **seamless integration** across the nanotechnology supply chain and hinders sustainability tracking.

- **Environmental Burden of IoT Devices**

IoT sensors and devices have their own carbon and material footprint**.** Producing and disposing of these devices could undermine sustainability unless designed with circular economy principles.

7. Future Directions of AI in Sustainable Nanotechnology

- **Autonomous Nano-Manufacturing Systems**

Fully automated nano-factories driven by AI models that adapt and optimize production in real time. For example use of reinforcement learning for dynamic process control of nanomaterial synthesis. It enhances resource efficiency and reduces human error in sustainable material production [26].

- **Green-by-Design AI Models**

AI used to design eco-friendly nanomaterials from the molecular level using predictive models. AI predicts environmental toxicity, biodegradability, and life cycle impact before physical synthesis [27].

- **Federated and Privacy-Preserving Learning**

  Collaborative AI development across industries and labs without sharing raw data, protecting IP. Nanotech companies use federated learning to train toxicity prediction models across sites [28].

- **Explainable AI for Nanotechnology**

  Increased adoption of interpretable AI to meet regulatory and safety standards in nano-production. It helps material scientists understand AI-generated recommendations for green chemistry [29].

- **Integration with Quantum Computing**

  Quantum-enhanced AI for simulating complex nanoscale behaviors with ultra-high accuracy.

  It revolutionizes material discovery by simulating interactions at atomic scale [30].

- **Edge AI for Real-Time Nano-Process Control**

Embedding AI on the edge (e.g., in sensors and embedded devices) for real-time control of nanofabrication processes. It reduces data transmission needs and latency; enhances energy efficiency and localized sustainability [31].

8. Future Directions of IoT in Sustainable Nanotechnology

- Nano-IoT (nIoT) Development

Ultra-miniaturized IoT sensors integrated directly into nanostructures and smart materials. In-situ monitoring of nanodevices and nanomaterials during real-world applications (e.g., biomedical implants or environmental sensors) [32].

- **Self-Powered and Energy-Harvesting IoT Devices**

Sustainable IoT sensors powered by nanogenerators (e.g., piezoelectric or thermoelectric materials). It enables long-term deployment of sensors without batteries, reducing e-waste [33].

- **IoT Devices for Real-Time Nano Process Control**

IoT devices integrated with on-chip AI (edge computing) for local data processing in real time. It reduces latency in controlling chemical reactions during nanoparticle synthesis [34].

- **Standardization and Interoperability Frameworks**

Development of global IoT interoperability standards specifically for nanotech applications. It facilitates communication between nano-factories, supply chains, and environmental monitors [35].

9. Future Directions of AI-IoT in Sustainable Nanotechnology

- **Digital Twins for Nano-Manufacturing**

Developing digital twins of nanomanufacturing systems using real-time IoT data and AI models. It enables predictive optimization, sustainability simulations, and virtual testing before physical implementation [36].

- **AI-IoT Integration for Sustainable Life Cycle Assessment (LCA)**

Automating Life Cycle Assessments of nano-products using AI algorithms fed with IoT-based real-time environmental data. It improves precision and scalability of LCA to support circular nanomanufacturing and regulatory compliance [37].

- **Blockchain + AIoT for Nano-Supply Chain Transparency**

Integrating blockchain with AI and IoT (AIoT) to enable secure, traceable, and ethical sourcing of nano-materials. It enhances trust and environmental accountability across global nanotech supply chains [38].

- **AI and IoT for Toxicity Prediction and Safer-by-Design Nanotech**

Using AI models (e.g., QSAR) trained on IoT-monitored environmental data to predict toxicity and ensure nanomaterials are "safe by design." It meets stringent regulatory standards and supports ethical sustainability frameworks [39].

- **AI and IoT Enabled Waste Reduction and Recycling Optimization**

AI systems analyzing IoT data to monitor and optimize waste reduction, recycling, and reuse of nanomaterials and by-products. It supports closed-loop manufacturing and material circularity [40].

10. Conclusion

AI and IoT are transforming sustainable nanotechnology by providing intelligent, data-driven solutions for material design, environmental monitoring, and lifecycle management. These technologies not only improve efficiency and safety but also ensure alignment with global sustainability goals. As research and innovation continue, the convergence of AI, IoT, and nanoscience will become a cornerstone of green technological development. Embracing interdisciplinary approaches and fostering regulatory clarity will be essential to realize the full potential of this transformative synergy. Though challenges exist especially in data, interpretability, and ethics; ongoing research and innovation are creating robust frameworks for AI to support a green nanotech future**.** However, it must be paired with green design principles and robust data governance to truly advance environmental goals.

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