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Review Article

Two heads are better than one: Unravelling the potential Impact of Artificial Intelligence in nanotechnology

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ABSTRACT

Artificial Intelligence (AI) and Nanotechnology are two cutting-edge fields that hold immense promise for revolutionizing various aspects of science, technology, and everyday life. This review delves into the intersection of these disciplines, highlighting the synergistic relationship between AI and Nanotechnology. It explores how AI techniques such as machine learning, deep learning, and neural networks are being employed to enhance the efficiency, precision, and scalability of nanotechnology applications. Furthermore, it discusses the challenges, opportunities, and future prospects of integrating AI with nanotechnology, paving the way for transformative advancements in diverse domains ranging from healthcare and materials science to environmental sustainability and beyond.

1. Introduction

The term artificial intelligence (AI) describes the development of systems that can be programmed to carry out tasks that are often assigned to human intelligence [1]. Natural language processing, deep learning neural networks, and machine learning algorithms are all included in AI. It is utilized in various fields, such as robotics [2], data mining [3], pattern/cue detection [4], and self-navigating devices [5], etc. The processing and administration of materials at the nanoscale, or size range between 1 and 100 nm, is referred to in terms of nanotechnology [6]. By combining different materials, tools, and systems, it produces those with novel qualities or attributes. Nanotechnology finds application in a variety of fields, such as diagnostics [7], electronics [8], therapeutics [9], sensing [10], theranostics [11], energy [12], and environmental remediation [13], where it offers solutions to health issues and clean energy generation challenges. The integration of AI with nanotechnology yields benefits in material design, fabrication process optimization, and the development of new, more accurate, and productive products. This is the way that science and technology will continue to advance and make new discoveries.

The significance and potential of AI and Nanotechnology are that their development can transform numerous spheres of human activity. AI's feature of analyzing large amounts of data, identifying patterns, and learning allows for the automation of various processes, and decision-making and problem-solving mechanisms across industries to improve industries and increase the efficiency and productivity thereof. Moreover, it is also used for a variety of individual assignments thanks to its ability to adapt: in healthcare, finance, etc., it ensures that the end result meets everyone's needs. Nanotechnology's potential is that nanomaterials can be created from raw materials that are manipulated at the atomic and molecular levels. Due to the unique properties and functions of these materials and devices, nanotechnology can be used to develop new killer technologies for the medicine, electronics, energy, and environmental sectors. It could be used to create targeted drug systems which will help reconstruct particularly aggressive and resistant cells more rapidly, make ultrahigh-efficient solar batteries, and perform divisions of dangerous contaminants [14].

But there are obstacles in both sectors. AI struggles with moral dilemmas, biased algorithms, and employment losses from automation. Nanotechnology faces regulatory hurdles, environmental effects, and safety issues. In order to fully utilize AI and nanotechnology and ensure their responsible and advantageous application for society, it is imperative that these challenges are addressed. Since AI and nanotechnology complement each other well and have the potential to work in concert to spur innovation and solve difficult problems, there is a driving force behind the exploration of their integration. While nanotechnology is precise in changing matter at the nanoscale, AI is able to evaluate large datasets and derive significant conclusions. Researchers hope to improve the performance, precision, and scalability of nanomaterial design, production processes, and device functionality by

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fusing AI methods like machine learning and neural networks with nanotechnology [15].

Furthermore, the interdisciplinary nature of nanotechnology and AI encourages cooperation between scientific fields, which results in the cross-pollination of concepts and approaches. This partnership makes it easier to develop cutting-edge solutions with broad applications in industries including energy, healthcare, and environmental sustainability. Additionally, combining AI with nanotechnology has the potential to address urgent social issues including environmental monitoring, renewable energy production, and disease diagnosis and treatment. Researchers can speed up the rate of discovery and innovation in nanotechnology by utilizing AI-driven methodologies, opening up new avenues for scientific study and technical innovations. The pursuit of game-changing solutions that advance sustainable development, raise human health, and improve quality of life is ultimately what drives research into the fusion of AI and nanotechnology.

2. Fundamentals of nanotechnology

The field of nanotechnology deals with the manipulation and control of matter on a very small scale, usually between one and one hundred nanometers [16]. Different from those at greater scales, materials of this scale have unique characteristics and behaviors. In a variety of industries, including electronics, medical, energy, and environmental science, nanotechnology refers to the creation, synthesis, characterization, and use of nanomaterials and nanodevices. Its range include the creation of new materials, manufacturing processes, and equipment with specialized features for particular uses, providing answers to problems in fields including environmental cleanup, renewable energy generation, and illness diagnosis and treatment.

By providing innovative methods for drug delivery [10], diagnostics [17], and treatment [9,18], the current uses of nanotechnology such as carbon dots in drug research are revolutionizing the healthcare services [19]. In order to improve patient outcomes, safety, and efficacy in medication delivery, a great deal of research and development is being done on nanoparticles, nanocarriers, and nanostructures. Targeted medication delivery, which minimizes off-target effects and lowers systemic toxicity, is made possible by nanotechnology. Drugs are encased into nanoparticles or nanocarriers that are intended to deliver therapeutic payloads to particular cells or tissues [20]. Drugs can be encapsulated in liposomes, polymeric nanoparticles, or dendrimers, and then delivered to specific areas within the body via these nanocarriers. Furthermore, nanotechnology makes it possible to develop formulations with controlled release, which precisely regulates the kinetics of drug release and maintains therapeutic concentrations for long periods of time. This increases patient compliance, lowers the frequency of dose, and improves therapeutic efficacy. Additionally, nanotechnology is essential in breaking down biological barriers like the blood-brain barrier, which makes it possible to transfer medications to the central nervous system for the treatment of neurological illnesses [21]. Fig. 1 depicts fundamentals of nanotechnology.

Apart from its application in drug delivery, nanotechnology is transforming drug discovery by enabling breakthroughs in high-throughput screening, personalized therapy, and nanoscale imaging. Real-time monitoring of drug distribution, pharmacokinetics, and therapy response is made possible by nanoparticles functionalized with targeting ligands and imaging agents. This allows for early illness detection and treatment optimization.

3. Fundamentals of Artificial Intelligence

In order to create machines that can mimic human intelligence and carry out tasks that normally need human cognition, AI is a revolutionary subject of computer science [1]. Fundamentally, it aims to mimic and mechanize cognitive processes like perception, learning, reasoning, and problem-solving. Natural language processing, robotics, computer vision, machine learning, neural networks, and other approaches are all included in it's broad category. A branch of AI called machine learning is concerned with creating algorithms that let computers learn from data and get better over time without the need for explicit programming. Applications of AI can be found in a wide range of industries, including healthcare, banking, entertainment, and transportation. AI-powered tools in healthcare can help with drug discovery, evaluate medical imaging, and forecast disease outcomes. AI algorithms are utilized in finance for automated customer care, algorithmic trading, and fraud detection. AI in transportation makes it possible for self-driving cars to navigate and make choices in challenging situations [22]. Fig. 2 shows various applications of AI.

Rapid advances in AI technologies have revolutionized industries and changed social standards, leading to successes in a number of sectors. AI has the ability to significantly enhance human abilities and spur creativity as it develops, paving the way for a time when intelligent robots will collaborate with people to tackle challenging issues and enhance quality of life. Large datasets encompassing chemical structures, biological experiments, and clinical data are analyzed by machine learning approaches in drug development to find patterns and linkages that conventional methods might miss [29]. By using known data to predict chemical activity against certain pharmacological targets or diseases, supervised learning algorithms like random forests and support vector machines can speed up the screening process and lower the cost of experiments.

Owing to its ability to extract complex properties from unprocessed data, deep learning, a subset of machine learning, has shown great promise in the drug development space [30]. To improve the accuracy of drug-target interactions, toxicity, and pharmacokinetics predictions, deep neural networks-in particular, convolutional neural networks (CNNs) and recurrent neural networks (RNNs)-are utilized to assess biological interactions, protein sequences, and chemical structures [31]. Especially well-suited for simulating intricate interactions in drug discovery datasets are neural networks, which draw inspiration from the structure and operation of the human brain. In order to facilitate the design of innovative drug candidates with desired attributes, these networks are able to learn nonlinear mappings between chemical traits and biological activity.

Virtual screening, lead optimization, and personalized medicine have advanced significantly as a result of the combination of deep learning, machine learning, and neural networks in drug development [32]. Researchers can speed up the process of identifying possible drugs, rank compounds for more testing, and tailor their properties for certain therapeutic uses by utilizing these AI tools. In the end, using AI to drug discovery has the potential to speed up the creation of safer, more efficient medicines for a variety of illnesses, which will help people and healthcare systems all around the world. A variety of AI applications for drug discovery are shown in Table 1.

4. Synergies between AI and nanotechnology

The combination of two revolutionary areas- AI and nanotechnology, has great potential to propel innovation and tackle difficult problems in a variety of fields. By combining the precision of nanotechnology with the computational capacity of AI to evaluate large datasets, new materials, gadgets, and systems with previously unheard-of capabilities can be generated [58].

The design and discovery of materials is one of the main domains where AI and nanotechnology converge. With the implementation of nanotechnology, materials can be engineered at the atomic and molecular level to have certain features, such as increased conductivity, reactivity, and strength. However, the design space for nanomaterials is large and intricate, and navigating it effectively requires the use of advanced computational tools. Additionally, researchers may investigate how nanomaterials behave in various settings and conditions by utilizing AI-driven computational modeling and simulation, which makes it easier to optimize the functionality and performance of

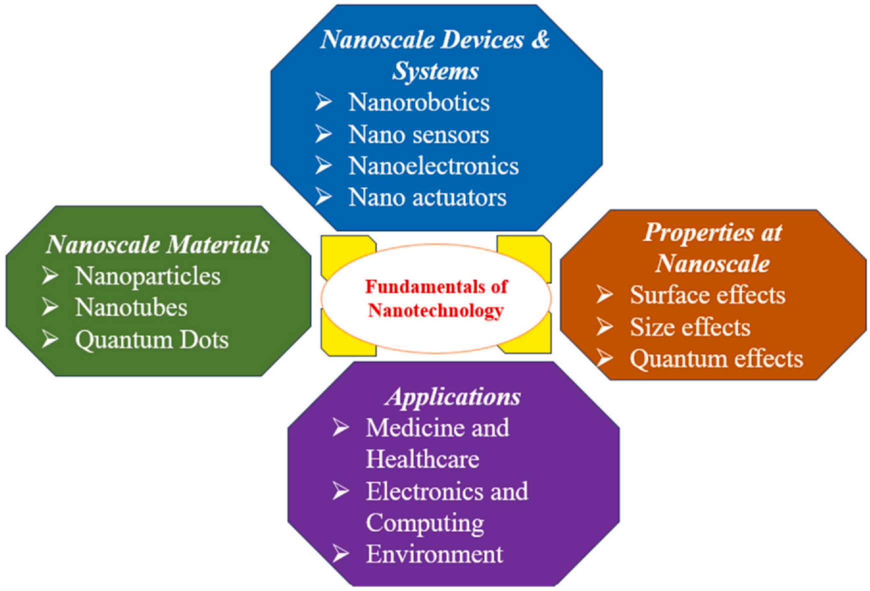

Fig. 1. Fundamentals of nanotechnology.

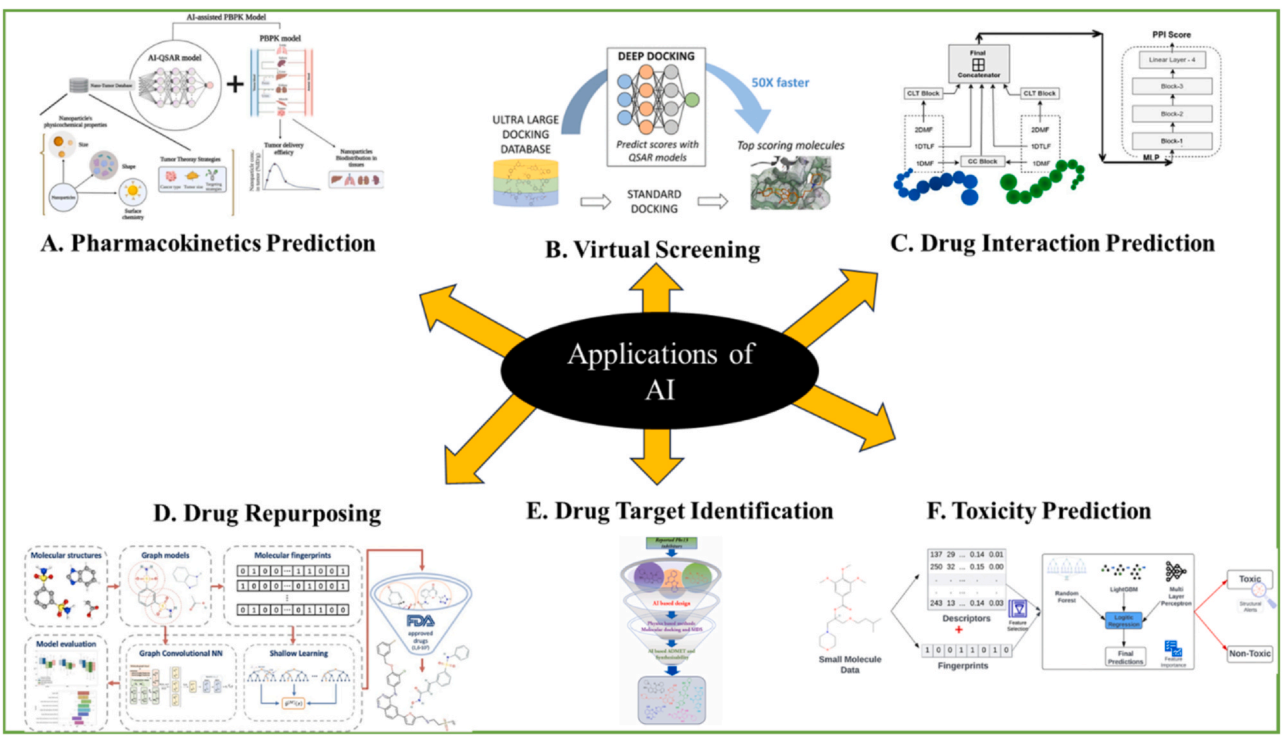

Fig. 2. Various applications of AI.
(a) (A) Application of AI in Pharmacokinetic Prediction (Reprinted with Permission from [23]. (b) (C) Application of AI in Drug Interaction Prediction (Reprinted with Permission from [25]. (c) (E) Application of AI in Drug Target Identification (Reprinted with Permission from [27]. (d) (B) Application of AI in Virtual screening (Reprinted with Permission from [24]. (e) (F) Application of AI in Toxicity prediction (Reprinted with Permission from [28]. (f) (D) Application of AI in Drug repurposing (Reprinted with Permission from [26].

materials. In addition to quickening the velocity of materials discovery, this cooperative approach improves our comprehension of nanoscale phenomena, which fosters the creation of novel materials with yet unheard-of qualities and uses.

The fields of nanofabrication and manufacturing are yet another field where AI and nanotechnology operate efficiently simultaneously [59]. For exact matter manipulation at the nanoscale, nanotechnology provides a range of fabrication methods, including bottom-up methods like self-assembly and top-down methods like lithography. To ensure the quality and reproducibility of the constructed nanostructures, these procedures, nevertheless, frequently call for precise control and supervision. These issues are addressed by AI-driven methods, which make it possible to monitor, control, and optimize processes in real time. Sensor data from nanofabrication processes can be analyzed by machine learning algorithms to identify anomalies, forecast faults, and adjust process parameters for increased productivity and efficiency. Additionally, AI-driven robotic systems can automate processes related to nanoassembly and manipulation, allowing for the high-throughput production of nanodevices and structures with previously unheard-of scalability and precision.

Table 1
Applications of Artificial intelligence (AI).

Application	Action	Reference
Virtual Screening	AI systems examine chemical structures to forecast how target proteins and drug candidates would interact, speeding up the process of finding possible leads.	[24,33,34]
Drug Target Identification	AI systems examine biological data, gene expression patterns, and protein-protein interaction networks, machine learning models are able to discover new therapeutic targets, leading to potential molecules.	[27,35,36]
Drug Repurposing	AI-driven methods examine the biological activity profiles and molecular structures of current medications to find novel therapeutic applications.	[26,37,38]
Biomarker Discovery	Genomics, proteomics, and metabolomics data are analyzed using machine learning algorithms to find biomarkers linked to disease diagnosis, prognosis, and therapy response.	[39–41]
Pharmacogenomics	AI methods evaluate genetic information to forecast a person's reaction to medication, allowing for customized treatment and the optimization of medication dosage schedules.	[42,43]
Toxicity Prediction	Through the analysis of chemical structures and biological features, machine learning models and neural networks are able to forecast the potential toxicity of medication candidates.	[28,44,45]
Pharmacokinetics Prediction	AI systems simulate how drugs are absorbed, distributed, metabolized, and excreted in order to forecast pharmacokinetic characteristics and enhance drug dosing regimens.	[23,46]
Drug Design and Optimization	Deep learning models enhance existing drugs for increased safety and efficacy and create new drug-like molecules with desired features.	[47,48]
Clinical Trial Optimization	AI-driven strategies streamline patient enrollment, data analysis, and clinical trial design to hasten drug development and cut expenses.	[49–51]
Drug Interaction Prediction	Medication safety is ensured by machine learning algorithms that forecast possible drug-drug interactions based on chemical structures, pharmacological characteristics, and patient data.	[25,52,53]
Risk Stratification	Precision medicine methods are made possible by AI tools that evaluate patient data to stratify populations based on prognosis, treatment response, and disease subtypes.	[54–57]

The combination of AI and nanotechnology in the field of nanomedicine shows great promise for transforming the paradigms of treatment and healthcare delivery [60]. Advanced drug delivery systems, diagnostic instruments, and therapies with improved imaging, targeting, and therapeutic capabilities have been made feasible by nanotechnology. Optimizing the safety and effectiveness of these nanomedical technologies, however, involves individualized strategies based on the unique traits and disease profiles of each patient. Precision medicine is made possible by AI-driven methods that stratify patient populations according to prognoses, treatment responses, and disease subtypes by evaluating vast amounts of patient data, including genomes, proteomics, and medical imaging. The best courses of action for individual patients can be chosen with the use of machine learning algorithms, which can detect biomarkers linked to drug response and illness progression. Furthermore, real-time drug administration, pharmacokinetic, and therapeutic response monitoring is made possible by AI-powered nanomedicine systems, which promotes flexible treatment plans and enhances patient outcomes.

The combination of AI with nanotechnology presents creative approaches to sustainability, remediation, and monitoring in environmental applications. Nanotechnology offers nanomaterials and nanosensors that can monitor environmental parameters, identify and eliminate contaminants, and facilitate the production of renewable energy. Nonetheless, the implementation of these nanotechnologies in actual environmental contexts necessitates the use of intelligent systems for resource optimization, data analysis, and decision-making. By offering data-driven insights and predictive models for environmental monitoring and management, AI-driven approaches help to address these issues. Through the analysis of sensor data from distributed networks of nanosensors, machine learning algorithms are able to anticipate pollutant concentrations, identify environmental contaminants, and optimize remediation procedures in real time. Additionally, the design and operation of nanomaterial-based energy systems, such solar cells and batteries, can be optimized for optimal efficiency and sustainability using AI-powered optimization algorithms [61]. Fig. 3 depicts synergies of Nanotechnology & AI.

The convergence of computational intelligence and nanoscale engineering is represented by the synergies between AI and nanotechnology, which promise transformational prospects across a variety of areas. Through the fusion of AI's computational prowess and nanotechnology's accuracy, scientists can better understand materials science, streamline nanofabrication procedures, transform healthcare delivery, and tackle urgent environmental issues.

4.1. Optimizing the design of nanomaterials

Computational modeling and simulation powered by AI is an effective means for comprehending intricate systems, forecasting behavior, and enhancing performance in a variety of domains, including materials science, engineering, healthcare, and environmental sustainability. This method makes use of AI computational capabilities, to analyze data, find patterns, and create predictive models that represent the dynamics of the system under study. The ability of AI-driven computational modeling and simulation to manage huge and heterogeneous datasets, such as theoretical predictions, simulation outputs, and experimental measurements, is one of its main advantages. With the use of machine learning algorithms, these datasets can be analyzed to find correlations, trends, and patterns that conventional analytical or empirical methods would miss. AI models may capture intricate linkages and nonlinear dynamics by learning from data, which leads to more precise predictions and insights into the behavior of the system being studied [63].

Furthermore, researchers may examine how systems behave in various contexts, settings, and parameters via AI-driven computational modeling and simulation, which makes it easier to conduct virtual experiments and test hypotheses. This virtual experimentation method eliminates the need for expensive and time-consuming experimental trials, which speeds up the discovery and optimization of materials, tools, and procedures. In materials research, for instance, AI models can direct the creation of novel materials with desired qualities, anticipate the attributes of hypothetical materials, and optimize material synthesis and processing settings for better performance [66].

AI-driven computer simulations enable real-time control and optimization of complex systems in addition to predictive modeling. Real-time sensor data from the system can be analyzed by machine learning algorithms, which can also be used to spot performance anomalies and modify control parameters for optimal system performance. In applications like advanced manufacturing, energy systems, and autonomous cars, where real-time modifications are essential for attaining desired outcomes and maintaining system integrity, this closed-loop feedback control technique is especially helpful. Furthermore, by offering a common framework for integrating data, models, and expertise from other areas, AI-driven computational modeling and simulation support interdisciplinary cooperation and knowledge integration. Through the integration of AI-powered data analytics with knowledge from the fields of engineering, biology, chemistry, and physics, scientists can

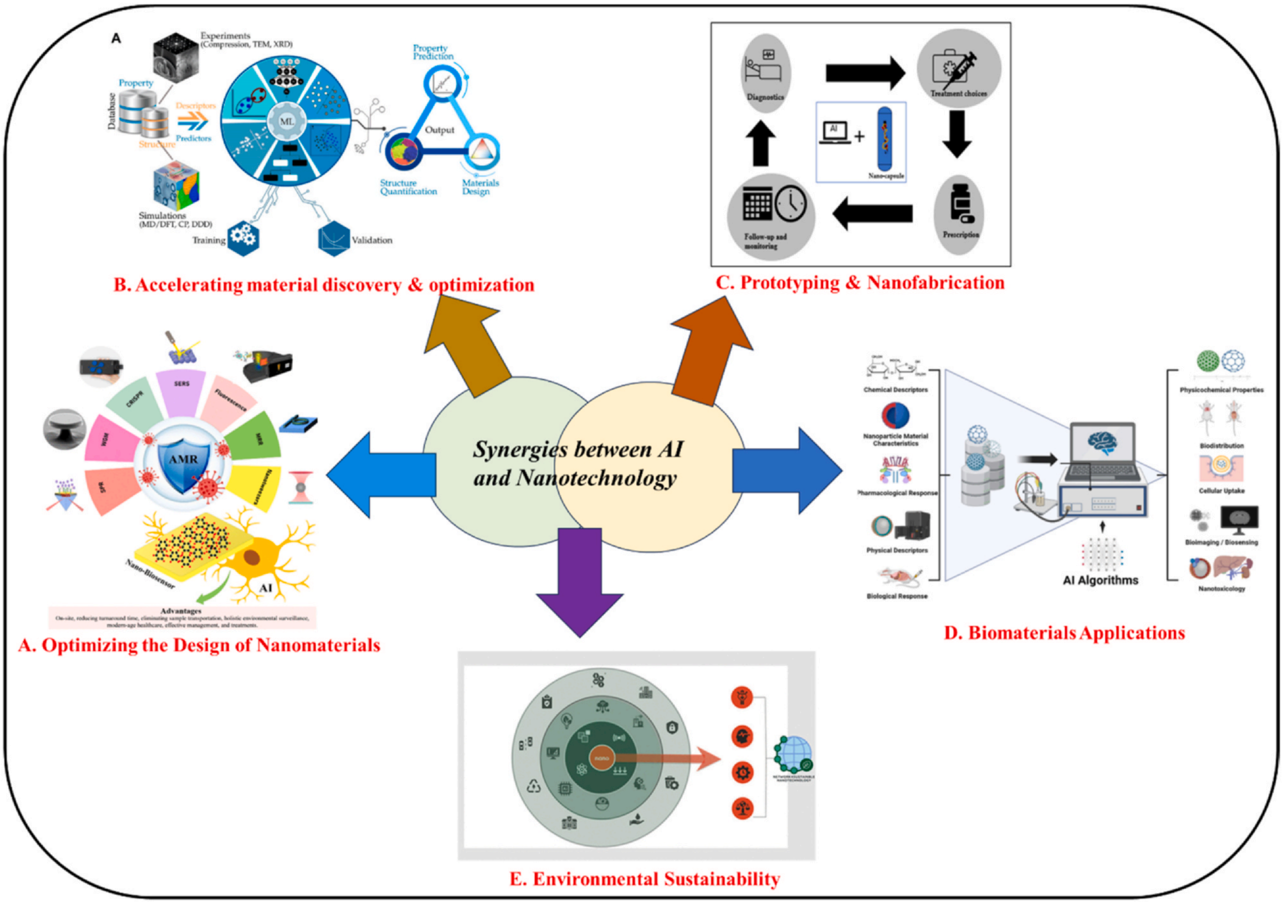

Fig. 3. Synergies of nanotechnology & AI (A) Optimizing the design of nanomaterials. (B) Accelerating material discovery & optimization. (C) Prototyping & nanofabrication. (D) Environmental sustainability. (E) Biomaterials applications.
(a) Reprinted with permission from [62]. (b) Reprinted with permission from [63]. (c) Reprinted with permission from [59]. (d) Reprinted with permission from [64]. (e) Reprinted with permission from [65].

create comprehensive models that represent the multifaceted and multiscale characteristics of complex systems, resulting in ground-breaking breakthroughs and discoveries [59].

Nanotechnology and Neural networks are strategic drivers for development of neuromorphic electronics. Emulation of neural networks is made possible by AI algorithms, which enhances the performance and usefulness of neuromorphic devices. The fabrication of materials and structures at the nanoscale level is made easier by nanotechnology, which is vital for producing parts with biomimetic qualities. When combined, they enable to build intelligent systems that simulate cognitive processes in the brain, opening up new possibilities in robotics and medical diagnostics [67].

4.2. Accelerating material discovery and optimization

AI plays a revolutionary role in material discovery and optimization for drug discovery by providing creative ways to find new drug candidates with improved safety and effectiveness profiles rapidly [68]. In order identify novel drug candidates, forecast their characteristics, and enhance their performance, researchers can examine enormous datasets of chemical compounds, biological assays, and clinical data using AI techniques like machine learning and deep learning. AI mostly uses predictive modeling and virtual screening to speed up material discovery for medication development. Large databases of biological activity data and molecular structure can be analyzed by machine learning algorithms to find compounds that may have medicinal promise. AI models can forecast the activity of hypothetical compounds against particular pharmacological targets or diseases by learning from patterns in the data. This capability helps to refine the search space and direct experimental efforts towards the most promising possibilities [69].

Furthermore, by anticipating the characteristics and behaviour of drug candidates in silico, AI-driven computational modeling and simulation aid in the optimization of drug candidates. In order to forecast the properties of novel compounds with structures comparable to existing ones, machine learning algorithms can examine the structure-property connections of known compounds. This method reduces the need for expensive and time-consuming experimental trials by allowing researchers to design and manufacture molecules with desirable qualities, such as enhanced potency, selectivity, and pharmacokinetic features [70].

AI enables the discovery of novel pharmacological targets and mechanisms of action using data-driven approaches, in addition to virtual screening and predictive modeling. Machine learning algorithms can find biomarkers linked to disease pathways and treatment responses by evaluating omics data, including proteomics, metabolomics, and genomes. This information helps guide the selection of the best drug targets and therapeutic approaches. Moreover, medication combinations and synergistic interactions that improve therapeutic efficacy and reduce drug resistance can be discovered by employing AI approaches. Moreover, enhancing medication efficacy and patient outcomes is greatly aided by AI-driven optimization of drug formulations and delivery methods. For personalized medicine approaches, machine learning algorithms can optimize drug dosage regimens and distribution channels by analyzing formulation data and patient-specific characteristics. Furthermore, the development of targeted drug delivery systems that improve drug delivery to certain tissues or cells while reducing off-target effects and systemic toxicity is made possible by AI-powered nanomedicine platforms [71,72].

4.3. Prototyping and nanofabrication

AI plays a critical role in nanofabrication and manufacturing by offering innovative methods to enhance scalability, accuracy, and efficiency in the development of nanoscale devices, materials, and structures [73]. AI tools facilitate the intelligent management, enhancement, and automation of nanofabrication procedures, resulting in revolutionary breakthroughs in a range of industries. Process control and monitoring is one of the main uses of AI in nanofabrication. To achieve desired results, precise control over factors like temperature, pressure, and chemical composition is necessary for nanofabrication procedures including lithography, etching, and deposition. AI-driven methods make it possible to monitor process variables in real-time, utilizing sensor data and feedback control mechanisms to optimize performance and modify process parameters. In order to identify anomalies, forecast process failures, and enhance process conditions for increased yield and quality of produced nanostructures, machine learning algorithms can evaluate sensor data.

Furthermore, by using predictive modeling and simulation, AI makes it easier to design and optimize nanofabrication processes. Machine learning algorithms are able to generate prediction models of the links between process, structure, and property by analyzing data from prior fabrication runs. With the use of these models, scientists can forecast how changes in a process will affect the characteristics of nanostructures that are created, which helps researchers create manufacturing procedures that are optimal for particular uses. AI-driven simulations also facilitate virtual experimentation, which speeds up the discovery and improvement of nanomaterials and devices by enabling researchers to investigate the behavior of nanostructures in various settings and conditions [74].

AI facilitates automation and robotics in nanofabrication and production, in addition to process optimization and monitoring. Robots driven by AI are able to operate and assemble complex objects at the nanoscale with previously unheard-of accuracy and efficiency [75]. These robotic systems use machine learning algorithms to learn from their experiences, adjust to changing conditions, and gradually improve performance. AI-driven robotics streamlines nanofabrication processes, lowers production costs, and boosts throughput by automating labor-intensive and repetitive operations. This allows for the scalable manufacture of nanoscale devices and materials for commercial applications. AI methods additionally render detection and quality monitoring in nanofabrication processes easier. In order to identify flaws, irregularities, and deviations from intended specifications, machine learning algorithms may analyze visuals and sensor data from fabricated nanostructures. AI-driven quality control remedies enable early intervention and corrective actions to increase yield and reliability in nanofabrication processes by detecting and characterizing flaws in real-time [59].

4.4. Biomaterials applications

AI is playing a revolutionary role in the design, optimization, and characterization of biomaterials with customized characteristics and functionalities for a broad range of biomedical applications [76,77]. For tissue engineering, regenerative medicine, drug delivery, and medical devices, researchers may find and produce novel biomaterials more quickly owing to AI's approaches including machine learning, deep learning, and neural networks.

AI plays a major role in the design and optimization of materials in biomaterials applications. In order to find correlations, trends, and patterns that inform the development of novel biomaterials, machine learning algorithms can examine huge databases of material properties, synthesis techniques, and performance measures. AI models can discover materials with desirable qualities, such mechanical strength, biocompatibility, and degradation kinetics, rapidly by learning from data and predicting the features of hypothetical materials, optimizing material compositions, and processing settings.

To further investigate the behavior of biomaterials at the molecular and nanoscale levels, researchers can utilize AI-driven computer modeling and simulation [78]. In order to forecast the biocompatibility, immunogenicity, and bioactivity of biomaterials, machine learning algorithms can examine molecular structures, protein-ligand interactions, and cellular reactions. AI models guide the development of biomaterials for particular biomedical applications by modelling the interactions between biomaterials and biological systems. These models shed light on the fundamental mechanisms driving host response, tissue regeneration, and cell-material interactions.

AI not only helps with material design but also optimizes biomaterials for tissue engineering and medication delivery applications. To optimize the design of drug delivery systems, such as hydrogels, microparticles, and nanoparticles, machine learning algorithms can examine cellular absorption pathways, diffusion mechanisms, and drug release kinetics. AI models facilitate the creation of more efficient and customized drug delivery systems for a range of therapeutic applications by forecasting the release profiles and targeting efficiencies of drug-loaded biomaterials [79]. AI methods also make it possible to characterize and monitor the quality of biomaterials at every stage of the production process. Machine learning algorithms are able to recognize errors, anomalies, and departures from intended specifications by analyzing image data, spectroscopic measurements, and mechanical tests. AI-driven quality control solutions guarantee the dependability, consistency, and security of biomaterials intended for clinical use by recognizing and measuring material attributes and performance indicators [80].

Medical practice is also being revolutionized by AI on several fronts. AI also uses image analysis for medical imaging, improves early warning of diseases by employing nanodevices, and accelerates the search for biomarkers for conditions like cancer. Additionally, AI transforms precision medicine by speeding up drug discovery through the prediction of protein structures and the construction of novel nanomolecules [81].

4.5. Environmental sustainability

Climate change and energy sustainability are major issues that need to be addressed, and one innovative way to do so is through AI-driven nanomaterial optimization for clean energy [82]. The discovery and development of nanomaterials with improved qualities for the generation, storage, and conversion of renewable energy can be sped up by researchers by utilizing AI techniques including machine learning, deep learning, and neural networks. Materials design and discovery are two of AI's main functions in the optimization of nanomaterials for sustainable energy. When designing new nanomaterials for energy applications, machine learning algorithms can find patterns, trends, and correlations by analyzing large datasets of material attributes, synthesis techniques, and performance measurements. AI models can accelerate the search for nanomaterials with desirable features like high efficiency, stability, and scalability by learning from data and predicting the properties of hypothetical materials, optimizing material compositions and processing conditions.

AI helps optimize devices and systems based on nanomaterials for sustainable energy applications, in addition to materials design. Energy device designs and operations, including those of photovoltaic cells, electrochemical cells, and catalytic reactors, can be optimized through the use of machine learning algorithms that evaluate sensor data, operating circumstances, and performance metrics. AI models help to create more dependable, economical, and efficient energy solutions by forecasting device performance under various operating settings and environmental situations. Nanomaterials can also be integrated into grid-scale applications' infrastructure and energy systems thanks to AI approaches. In order to optimize the deployment and operation of nanomaterial-based energy technologies, such as energy storage systems, smart grids, and renewable energy integration solutions, machine learning algorithms can assess data on renewable energy sources, grid stability, and patterns of energy consumption. AI-driven energy management systems facilitate the efficient use of renewable energy resources and the shift to a sustainable energy future by offering real-time insights and predictive analytics [83,84].

As a very sensitive, selective, and real-time means of detecting pollutants and toxins in air, water, soil, and food, nanosensors provide a promising new paradigm for environmental monitoring and pollution control. The exceptional characteristics of nanomaterials, including their high surface-to-volume ratio, quantum effects, and surface reactivity, are utilized by these miniature sensors to achieve previously unheard-of levels of accuracy and efficiency for detecting and measuring minuscule amounts of environmental contaminants. Nanosensors' excellent sensitivity to a variety of chemical and biological analytes is one of its main advantages for environmental monitoring [85].

Through a variety of processes, including surface adsorption, chemical reaction, and optical transduction, nanomaterials with inherent features, such as carbon nanotubes, graphene, metal nanoparticles, and quantum dots, allow for the selective detection of particular contaminants. Nanosensors are able to bind to target analytes selectively, even at low concentrations, by functionalizing nanomaterials with particular receptors, ligands, or biomolecules. This allows for highly sensitive and specific detection [86].

Furthermore, nanosensors provide continuous, on-site environmental parameter measurement without the requirement for sample collection and laboratory analysis thanks to their real-time monitoring capabilities. Nanomaterials have been made smaller and more integrated into portable sensor platforms, making them deployable in hard-to-reach places. This allows for real-time monitoring of environmental pollution and the creation of early warning systems for possible threats. Moreover, remote data transmission and monitoring are made possible by wireless connectivity and data processing power, which empowers stakeholders to respond quickly and decisively to reduce environmental concerns. Nanosensors are perfect for distributed sensing networks and wearable devices for personal exposure monitoring since they are small, inexpensive, and have excellent sensitivity and real-time monitoring capabilities. Nanosensors can be incorporated into small, reasonably priced devices for widespread use in industrial, agricultural, and urban environments by utilizing advancements in microfabrication, nanotechnology, and wireless communication. This will enable for thorough monitoring of environmental pollution and its effects on ecosystems and human health.

Monitoring air quality and reducing pollution is one of the main uses of nanosensors in environmental monitoring [87]. Nanosensors possess the ability to identify a broad spectrum of air pollutants with exceptional sensitivity and specificity, such as carbon monoxide (CO), sulfur dioxide (SO_2), nitrogen oxides (NOx), particulate matter (PM), and volatile organic compounds (VOCs). Nanosensors allow for real-time monitoring of air quality, enabling us to improve air quality and safeguard human health by identifying pollution sources, assessing exposure risks, and implementing mitigation measures. Moreover, heavy metals, pesticides, medications, pathogens, and other contaminants can be detected in wastewater and water bodies by using nanosensors for pollution management and water quality monitoring. Nanosensors provide real-time monitoring of water quality indicators, which facilitates the early detection of pollution events, trend analysis, and remediation strategy implementation to safeguard aquatic ecosystems and potable water sources [88,89].

5. Challenges and future prospects

AI in nanotechnology has enormous potential, but there are a number of obstacles and restrictions that need to be overcome before successful application and integration can occur. First and foremost, a lot of data is needed for AI algorithms' training and validation. However, because of the complexity and diversity of nanomaterials and processes, it can be difficult to gather big and high-quality datasets in nanotechnology. The creation of reliable and accurate AI models may be hampered by the lack of data. Collaboration between specialists in a variety of disciplines, including computer science, chemistry, materials science, and physics, is necessary for AI in nanotechnology. There are communication, coordination, and knowledge transfer issues when bridging the gap between various fields and integrating diverse skills. Fig. 4 depicts merits and limits of AI & nanotechnology.

Deep learning neural networks and other AI models used in nanotechnology are frequently complicated and opaque, making it challenging to understand the decision-making process [90]. The trust and acceptability of AI-driven predictions and insights are restricted by

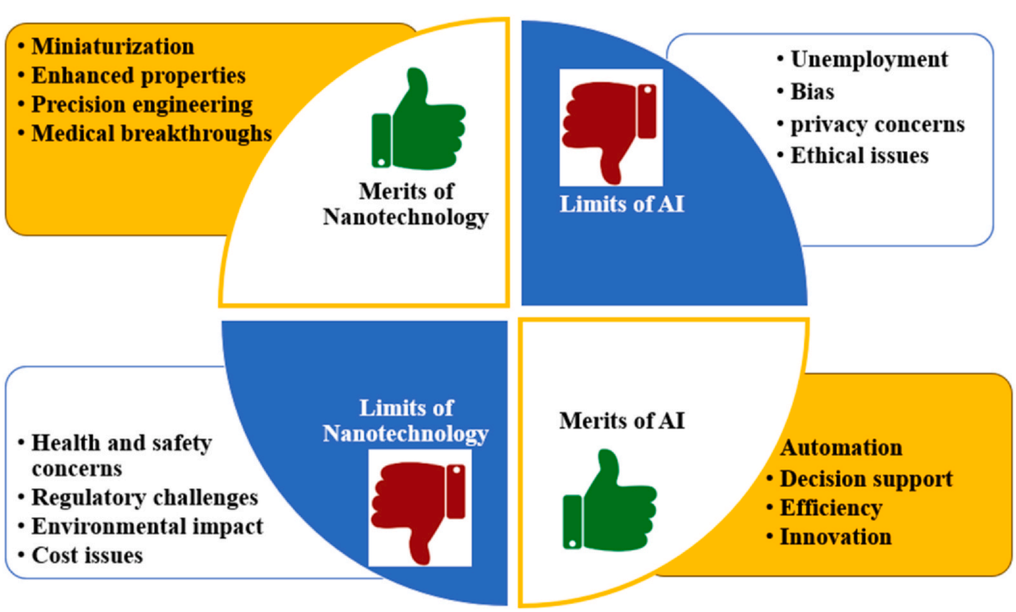

Fig. 4. Merits and limits of AI & nanotechnology.

their lack of interpretability, particularly in crucial applications like drug research and healthcare. For training and inference, AI algorithms-especially deep learning models-need a substantial amount of processing power. Large datasets and complicated models can put a strain on computational infrastructure, causing problems with scalability and performance, particularly in environments with limited resources like labs and research centers. Concerns about data privacy, security, prejudice, and responsibility are among the ethical and legal issues that are brought up by the use of AI in nanotechnology.

Maintaining public confidence in AI-driven nanotechnology applications requires ensuring fairness, openness, and adherence to regulatory norms. AI models may find it difficult to generalize to new data or domains if they were trained on certain datasets or tasks. Techniques like transfer learning, domain adaptation, and ensemble approaches are necessary to achieve robustness and generalization, but they may present difficulties in nanotechnology because of the complexity and diversity of materials and processes involved. The creation and implementation of AI-driven nanotechnology solutions may necessitate a large investment in software tools, infrastructure, and knowledge. Access to AI technology may be restricted by high costs and technological obstacles, especially for academics and organizations with insufficient funding or experience. The large use of AI in nanotechnology poses issues with inequality, autonomy, and job displacement that have wider societal ramifications. The effects of AI-driven technologies on people, communities, and society at large must be carefully considered in order to address these ethical and societal issues.

In order to create unique nano-molecular structures with desirable features for drug development, researchers are employing deep generative models called Generative Adversarial Networks, or GANs. Generating diverse and unique chemicals that are expected to display specific biological activities, such attaching to a target protein or influencing a biological pathway, is made possible by researchers training GANs on enormous databases of chemical compounds and their accompanying features. Exploration of chemical space and lead compound discovery for drug development are expedited by this AI-driven methodology [91].

Deep learning models, such as convolutional neural networks (CNNs) and recurrent neural networks (RNNs), are being used to predict the activity of nanomaterials against therapeutic targets or disease pathways for the purposes of Virtual Screening and Compound Prioritization. These AI models can shorten the time and expense involved with conventional high-throughput screening techniques by ranking possible drug candidates for experimental validation based on their analysis of biological data and molecular structures. Researchers can quickly find intriguing lead compounds with medicinal potential by using AI-powered virtual screening.

Quantitative Structure-Activity Relationship (QSAR) Models use machine learning techniques to predict nanomaterials/chemical compounds' biological activity based on their structural properties, with the goal of predictive modeling for drug optimization [92]. Through the utilization of QSAR models, researchers can enhance the potency, selectivity, and pharmacokinetics of lead compounds by examining the correlations between molecular descriptors and biological activities. With the help of AI, drug candidates are rationally designed, speeding up the process of drug optimization and raising the possibility of successful clinical trials.

AI-driven network-based methods for polypharmacology and drug repurposing incorporate a variety of data sources, such as chemical, biological, and clinical data, to find novel therapeutic uses for already-approved medications [93,94]. These methods can forecast the effectiveness of current medications for novel indications and identify possible drug-disease connections by examining drug-target interaction networks and illness networks. This AI-powered approach makes it possible to quickly identify medications that can be used for different purposes and investigate the impacts of polypharmacology, which can result in the development of novel therapeutic approaches for a range of illnesses.

AI-driven advancements in nanotechnology for drug discovery enable the development of more individualized and efficient medications, which improves patient outcomes and care. The precise and controlled administration of treatments to diseased tissues or cells has been rendered feasible by targeted drug delivery systems and nanomedicine platforms, which also minimize off-target effects and lower patient side effects. AI and nanotechnology-driven advanced diagnostic tools and imaging techniques improve disease detection, monitoring, and treatment response assessment, resulting in earlier diagnosis and improved disease management. AI has the potential to revolutionize materials science and engineering through the design and optimization of customized properties for a wide range of applications in nanotechnology. The development of innovative materials with improved performance properties-such as mechanical strength, electrical conductivity, and thermal stability-for use in electronics, energy storage, and aerospace is accelerated by computational materials design methodologies. AI approaches have facilitated the development of nanomaterials-based sensors and actuators that facilitate the creation of materials systems that are both responsive and adaptive. These materials find application in robotics, smart materials, and biomedical devices [95,96].

5.1. Challenges in merging AI and nanotechnology

AI technologies such as Quantitative Structure-Activity Relationship (QSAR) models, Convolutional Neural Networks (CNNs), and Generative Adversarial Networks (GANs) provide considerable advantages in nanotechnology research. Nonetheless, a number of obstacles still need to be overcome in order to fully realize AI's promise for improving nanotechnology. For instance, in order to train efficiently, AI models need a lot of high-quality data. Due to restrictions in experimental methods and data collection procedures, it might be difficult to obtain enough data in nanotechnology, particularly at the nanoscale [97,98]. But this may be avoided with the aid of methods like data augmentation and transfer learning, which enhance AI models even in the face of minimal datasets [99].

Second, considering nanoscale phenomena like surface contacts and quantum effects are distinct from larger-scale phenomena, directly applying typical AI algorithms to nanotechnology challenges could fail to deliver the most promising results [100,101]. Therefore, new AI approaches can handle complicated nanoscale data and interactions more efficiently, such as constructing new algorithms or utilizing reinforcement learning for nanorobotics [102]. Third, there aren't enough comprehensive regulatory frameworks in place to handle the unique problems that AI-integrated nanotechnologies offer. Furthermore, as AI applications in nanotechnology develop, moral questions about security, privacy, and the appropriate deployment of AI-driven technology surface [103]. To build standards to ensure the safe, transparent, and ethical deployment of AI technologies in nanotechnology, strong ethical principles and regulatory frameworks must be established [104,105]. Fourth, integrating AI technology into nanotechnology research may be too expensive, particularly for smaller labs or organizations with fewer resources [64]. Access to the sophisticated computational resources required for AI modeling and training can also be a hindrance. In these situations, agencies might investigate AI-driven nanotechnology research efforts with passion and confidence with the support of fundings, cloud-based services, and open-access platform promotion. While there is great promise for revolutionary innovation across many areas when AI and nanotechnology are combined, resolving the aforementioned obstacles is essential to achieving this potential in a safe and responsible manner.

6. Conclusion

A revolutionary paradigm shift with broad ramifications for companies and scientific fields is represented by the combination of AI with nanotechnology. AI -driven nanotechnology is transforming patient care and disease management by speeding up the development of tailored medications and focused therapies. AI -driven advancements in nanotechnology have a positive impact on materials science and engineering by facilitating the creation of customized characteristics for a wide range of applications, including electronics and aerospace. In addition, artificial intelligence-enabled clean energy technologies and nanosensors provide ways to reduce pollution and combat climate change, paving the way for a more sustainable future in environmental monitoring and sustainability. Attempting to illuminate the rapidly developing field of AI and nanotechnology, this review hopes to pave the way for revolutionary developments in science, technology, and society by showcasing their complementary potential. We may explore new creative avenues and tackle the most important issues confronting humanity in the twenty-first and future centuries by using a multidisciplinary approach and leveraging AI to enhance and develop nanotechnology.

Ethics approval and consent to participate

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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