Nano Nexus & Applications

www.nna.reapress.com

Nano. Nex. App. Vol. 1, No. 3 (2026) 178–198.

Paper Type: Original Article

Artificial Intelligence and Machine Learning in Functional Nanomaterials: From Materials Discovery to Industrial Applications

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Citation:

Received: 25 September 2025 *Revised: 04 January 2026* *Accepted: 19 March 2026*	Pourqasem, J. (2026). Artificial intelligence and machine learning in functional nanomaterials: From materials discovery to industrial applications. *Nano Nexus & Applications, 1*(3), 178-198.

Abstract

Artificial Intelligence (AI), particularly Machine Learning (ML), has emerged as a transformative technology in nanomaterials research by enabling data-driven materials discovery, design, characterization, and optimization. The integration of ML with experimental techniques, computational modeling, and materials databases has significantly accelerated the development of advanced nanomaterials while reducing the time, cost, and complexity associated with conventional trial-and-error approaches. This review provides a comprehensive overview of recent advances in ML applications across the entire nanomaterial development pipeline. Fundamental ML paradigms, including supervised, unsupervised, reinforcement, and Deep Learning (DL), are first introduced, followed by their applications in nanomaterial discovery, property prediction, and synthesis optimization. Emerging AI-driven strategies such as High-Throughput Screening (HTS), inverse design, Graph Neural Networks (GNNs), and generative AI are also discussed as promising approaches for accelerating the development of next-generation functional nanomaterials. Furthermore, recent progress in AI-assisted nanomaterial characterization, energy-related nanomaterials, environmental nanotechnology, nanoelectronics, smart sensors, and intelligent manufacturing is critically reviewed. The current challenges associated with data availability, model interpretability, generalization capability, and experimental validation are also highlighted, together with future research directions involving explainable AI, autonomous laboratories, digital twins, and foundation models. This review demonstrates that ML has evolved from a predictive computational tool into a key enabling technology for intelligent nanomaterials research. Continued advances in algorithms, data infrastructure, and interdisciplinary collaboration are expected to accelerate the development of sustainable, high-performance nanomaterials for diverse scientific, industrial, energy, and environmental applications.

Keywords: Machine learning, Artificial intelligence, Nanomaterials, Materials informatics, Property prediction, Autonomous materials discovery, Generative artificial intelligence.

1 | Introduction

Nanotechnology has emerged as one of the most rapidly evolving scientific disciplines of the twenty-first century, driving significant advances across materials science, electronics, energy, environmental engineering,

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https://doi.org/10.48314/nna.vi.70

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and industrial manufacturing [1–3]. Owing to their unique physicochemical properties, nanomaterials exhibit superior mechanical strength, enhanced electrical and thermal conductivity, large specific surface area, and remarkable catalytic activity compared with their bulk counterparts. These exceptional characteristics have enabled the development of high-performance materials for applications ranging from energy storage systems and environmental remediation to nano sensors, nanoelectronics, and advanced functional coatings [4].

Recent progress in nanomaterials research has resulted in the development of a wide variety of functional materials, including metallic nanoparticles, carbon-based nanomaterials, metal oxides, quantum dots, Metal Organic Frameworks (MOFs), and polymer nanocomposites. Although these materials have demonstrated outstanding performance in numerous applications, their design and optimization remain highly challenging [5–7]. The functional properties of nanomaterials are strongly influenced by multiple interconnected factors, including chemical composition, particle size, morphology, crystal structure, synthesis conditions, and surface chemistry. Consequently, identifying the optimal combination of these parameters through conventional experimental approaches is often expensive, labor-intensive, and time-consuming [8–10].

To address these challenges, computational techniques have become increasingly important in nanomaterials research. Conventional simulation methods such as Density Functional Theory (DFT), Molecular Dynamics (MD), and finite element analysis have significantly improved the understanding of nanoscale phenomena. However, these approaches frequently require substantial computational resources and are often impractical for exploring the enormous design space associated with modern functional nanomaterials [11].

In recent years, Machine Learning (ML) has emerged as a powerful data-driven approach capable of accelerating nanomaterials research. Unlike traditional computational methods, ML algorithms learn complex relationships directly from experimental and computational data, enabling rapid prediction of material properties, optimization of synthesis parameters, automated analysis of characterization data, and discovery of novel nanomaterials. The integration of ML with high-throughput experiments, advanced simulations, and large materials databases has established a new paradigm known as materials informatics, which is transforming the way functional nanomaterials are designed and optimized [12–15].

ML has already demonstrated considerable success in predicting thermal, mechanical, electrical, optical, and catalytic properties of nanomaterials while significantly reducing the time and cost associated with conventional trial-and-error experimentation. Furthermore, recent advances in Deep Learning (DL), Explainable Artificial Intelligence (XAI), and autonomous laboratories are enabling intelligent materials discovery and real-time process optimization, opening new opportunities for industrial-scale nanomaterial development [11].

Despite these remarkable achievements, several challenges remain before ML can be fully integrated into nanomaterials research. Limited availability of high-quality datasets, lack of standardized databases, model interpretability, data reproducibility, and generalization across different material systems continue to restrict the broader adoption of AI-driven methodologies. Addressing these challenges requires interdisciplinary collaboration among materials scientists, chemists, computer scientists, and data engineers [16–18].

This review provides a comprehensive overview of recent advances in the application of ML to functional nanomaterials. It discusses the fundamental concepts of ML, its role in nanomaterial discovery, property prediction, synthesis optimization, and materials characterization, together with current industrial applications, existing challenges, and future research directions. By summarizing recent developments and emerging trends, this review aims to provide researchers with a comprehensive perspective on the growing convergence of Artificial Intelligence (AI) and nanotechnology.

2 | Machine Learning in Nanomaterials: Fundamental Concepts

ML has become one of the fundamental enabling technologies driving the digital transformation of nanomaterials research. By integrating advanced computational algorithms with experimental data, theoretical modeling, and materials databases, ML provides powerful tools for understanding complex structure property

relationships, predicting material performance, and accelerating materials discovery [19]. To establish the foundation for the subsequent sections, this chapter first introduces the evolution of ML in materials science, followed by the major categories of ML algorithms, DL techniques, and the growing role of materials databases in supporting data-driven nanomaterials research.

2.1 | Evolution of Machine Learning in Materials Science

The rapid advancement of nanotechnology has led to an exponential increase in experimental and computational data, fundamentally transforming the way functional nanomaterials are designed, synthesized, and optimized. Modern characterization techniques, including Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM), X-ray Diffraction (XRD), Raman spectroscopy, and X-ray Photoelectron Spectroscopy (XPS), together with computational approaches such as DFT and MD simulations, generate enormous amounts of high-dimensional data describing the structural, chemical, thermal, electrical, and mechanical characteristics of nanomaterials. While these datasets contain valuable information regarding structure property relationships, extracting meaningful knowledge using conventional statistical methods has become increasingly challenging [18–21].

Historically, the development of advanced nanomaterials relied primarily on empirical trial-and-error experimentation supported by theoretical modeling. Researchers systematically modified synthesis parameters, including precursor composition, reaction temperature, synthesis duration, pH, and processing conditions, to achieve materials with desired functional properties. Although this approach has significantly contributed to the development of nanotechnology, it is often labor-intensive, time-consuming, and economically inefficient due to the enormous design space associated with functional nanomaterials [22].

The emergence of computational materials science partially addressed these limitations by enabling atomistic and multiscale simulations capable of predicting material behavior before experimental validation. However, high-fidelity computational techniques remain computationally demanding and are generally unsuitable for rapidly exploring the vast combinations of chemical compositions, nanostructures, and processing parameters encountered in contemporary materials research.

The recent integration of ML into materials science has introduced a paradigm shift from conventional physics-driven methodologies toward data-driven materials discovery. Rather than relying exclusively on explicit mathematical models, ML algorithms identify complex nonlinear relationships directly from experimental observations, computational simulations, and large-scale materials databases. This capability enables rapid prediction of material properties, optimization of synthesis parameters, automated analysis of characterization data, and accelerated identification of promising nanomaterials with targeted functionalities [21–23].

This convergence has given rise to the emerging discipline of materials informatics, which combines materials science, AI, data science, and computational modeling to accelerate the development of advanced materials. In nanomaterials research, ML has been successfully applied to diverse tasks, including property prediction, nanomaterial classification, synthesis optimization, image analysis, defect identification, catalyst discovery, and intelligent process control. Consequently, ML has evolved from a supporting computational technique into a key enabling technology for next-generation nanomaterials research, facilitating faster innovation while substantially reducing experimental costs and development time [22].

2.2 | Categories of Machine Learning

ML algorithms are generally categorized according to the type of learning strategy employed and the availability of labeled data. The four principal categories include supervised learning, unsupervised learning, semi-supervised learning, and Reinforcement Learning (RL). Although these approaches differ in their underlying methodologies, each provides unique capabilities for addressing specific challenges in nanomaterials research [23]. A comparative summary of the major ML paradigms, their representative algorithms, advantages, limitations, and typical applications in nanomaterials research is presented in *Table 1*.

Table 1. Comparison of major machine learning paradigms and their applications in nanomaterials research.

Learning Paradigm	Learning Strategy	Typical Algorithms	Representative Applications in Nanomaterials	Main Advantages	Limitations
Supervised learning	Learns from labeled datasets	Linear Regression (LR), SVM, Random Forest (RF), XGBoost, ANN	Property prediction, thermal conductivity estimation, mechanical property prediction, catalyst performance	High prediction accuracy; straightforward implementation	Requires large labeled datasets
Unsupervised learning	Discovers hidden patterns without labels	K-means, Hierarchical Clustering, PCA, t-SNE, UMAP	Nanomaterial clustering, morphology classification, dimensionality reduction	Identifies hidden relationships; useful for exploratory analysis	Results may be difficult to interpret
Semi-supervised learning	Combines labeled and unlabeled data	Self-training, Graph-based learning, Pseudo-labeling	Image classification, limited-data property prediction	Reduces dependence on labeled datasets	Sensitive to label quality
Reinforcement learning	Learns through interaction with an environment	Q-learning, Deep Q Networks (DQN), Policy Gradient (PG)	Autonomous synthesis optimization, intelligent process control, robotic experimentation	Adaptive optimization and decision making	Computationally intensive and still emerging in nanomaterials

2.2.1 | Supervised learning

Supervised learning is the most widely adopted ML approach in nanomaterials research. In this paradigm, algorithms are trained using labeled datasets in which input variables (features) are associated with known output variables (target properties). The objective is to establish predictive relationships that enable accurate estimation of material properties for previously unseen samples [24], [25]. Typical input features include chemical composition, particle size, morphology, crystal structure, synthesis conditions, and computational descriptors, whereas target variables may represent thermal conductivity, electrical conductivity, catalytic activity, adsorption capacity, mechanical strength, or optical characteristics. Common supervised learning algorithms include Linear Regression (LR), Support Vector Machines (SVM), Random Forests (RF), Gradient Boosting (GB) methods, and Artificial Neural Networks (ANNs), all of which have demonstrated excellent predictive capability in nanomaterials research.

2.2.2 | Unsupervised learning

Unlike supervised learning, unsupervised learning operates without labeled datasets and seeks to identify hidden structures or intrinsic patterns within complex data. These techniques are particularly valuable for clustering nanomaterials with similar characteristics, identifying anomalous observations, reducing data dimensionality, and exploring relationships that may not be evident through conventional statistical analysis. Frequently employed unsupervised learning methods include K-means clustering, hierarchical clustering, Principal Component Analysis (PCA), t-distributed Stochastic Neighbor Embedding (t-SNE), and Uniform Manifold Approximation and Projection (UMAP). These algorithms facilitate visualization of high-dimensional datasets and support knowledge discovery in nanomaterials research [26].

2.2.3 | Semi-supervised learning

Semi-supervised learning combines a limited number of labeled samples with a substantially larger collection of unlabeled data. This approach is particularly attractive in nanomaterials research because acquiring experimentally labeled datasets is often expensive and time-consuming. By utilizing both labeled and unlabeled information, semi-supervised algorithms improve prediction performance while reducing dependence on extensive experimental measurements [12].

2.2.4 | Reinforcement learning

RL differs from conventional learning paradigms by enabling an intelligent agent to learn optimal decisions through continuous interaction with its environment. Instead of relying on predefined labels, the algorithm receives feedback in the form of rewards or penalties and gradually improves its decision-making strategy. In nanomaterials research, RL has recently attracted considerable attention for autonomous materials discovery, robotic experimentation, adaptive process optimization, and intelligent manufacturing systems [17].

2.3 | Deep Learning in Nanomaterials

DL, a specialized branch of ML based on multilayer ANNs, has become one of the most influential technologies in modern nanomaterials research. Unlike conventional ML algorithms that often require manual feature engineering, DL models automatically extract hierarchical representations from raw data, enabling superior performance in handling highly complex and high-dimensional datasets. Recent advances in DL have significantly enhanced the automated analysis of microscopy and spectroscopy data. Convolutional Neural Networks (CNNs) have demonstrated remarkable success in interpreting SEM, TEM, AFM, and optical microscopy images, enabling automated particle segmentation, morphology classification, defect detection, and phase identification. Similarly, Recurrent Neural Networks (RNNs), Graph Neural Networks (GNNs), and transformer-based architectures have expanded the capability of DL for predicting material properties, modeling atomic structures, and discovering novel nanomaterials. Despite these advantages, DL models generally require large, high-quality datasets and substantial computational resources for effective training. Consequently, improving data availability, model interpretability, and computational efficiency remains an active area of research in AI-driven nanomaterials science [26–28].

2.4 | General Workflow of ML-Based Nanomaterials Research

The successful application of ML in nanomaterials research generally follows a systematic workflow that integrates experimental observations, computational simulations, and data-driven modeling. Although specific methodologies vary according to the research objective, most studies include several common stages.

The workflow begins with data acquisition, where experimental measurements, computational simulations, literature databases, and publicly available materials repositories provide the raw information required for model development. Widely used databases include Materials Project, AFLOW, OQMD, NOMAD, JARVIS, and NanoMine, which collectively provide extensive datasets describing structural, electronic, mechanical, thermal, and chemical properties of diverse material systems. Following data collection, data preprocessing and feature engineering are performed to eliminate inconsistencies, normalize variables, address missing values, and identify descriptors that effectively represent material characteristics. Appropriate feature selection is essential for improving model accuracy while reducing computational complexity [24].

The processed dataset is subsequently divided into training, validation, and testing subsets before selecting an appropriate ML algorithm according to the target application. Model performance is commonly evaluated using statistical metrics such as the coefficient of determination (R^2), Mean Absolute Error (MAE), Root Mean Square Error (RMSE), accuracy, precision, recall, and F1-score, depending on whether the task involves regression or classification. Finally, the validated model is applied to predict material properties, optimize synthesis parameters, identify promising candidate materials, or guide future experimental investigations. This iterative workflow enables continuous refinement of predictive models as additional experimental and computational data become available, thereby accelerating the discovery and optimization of advanced functional nanomaterials.

Fig. 1 summarizes the general workflow of ML-based nanomaterials research, highlighting the major stages involved in data acquisition, preprocessing, feature engineering, model development, validation, and practical implementation [26–29].

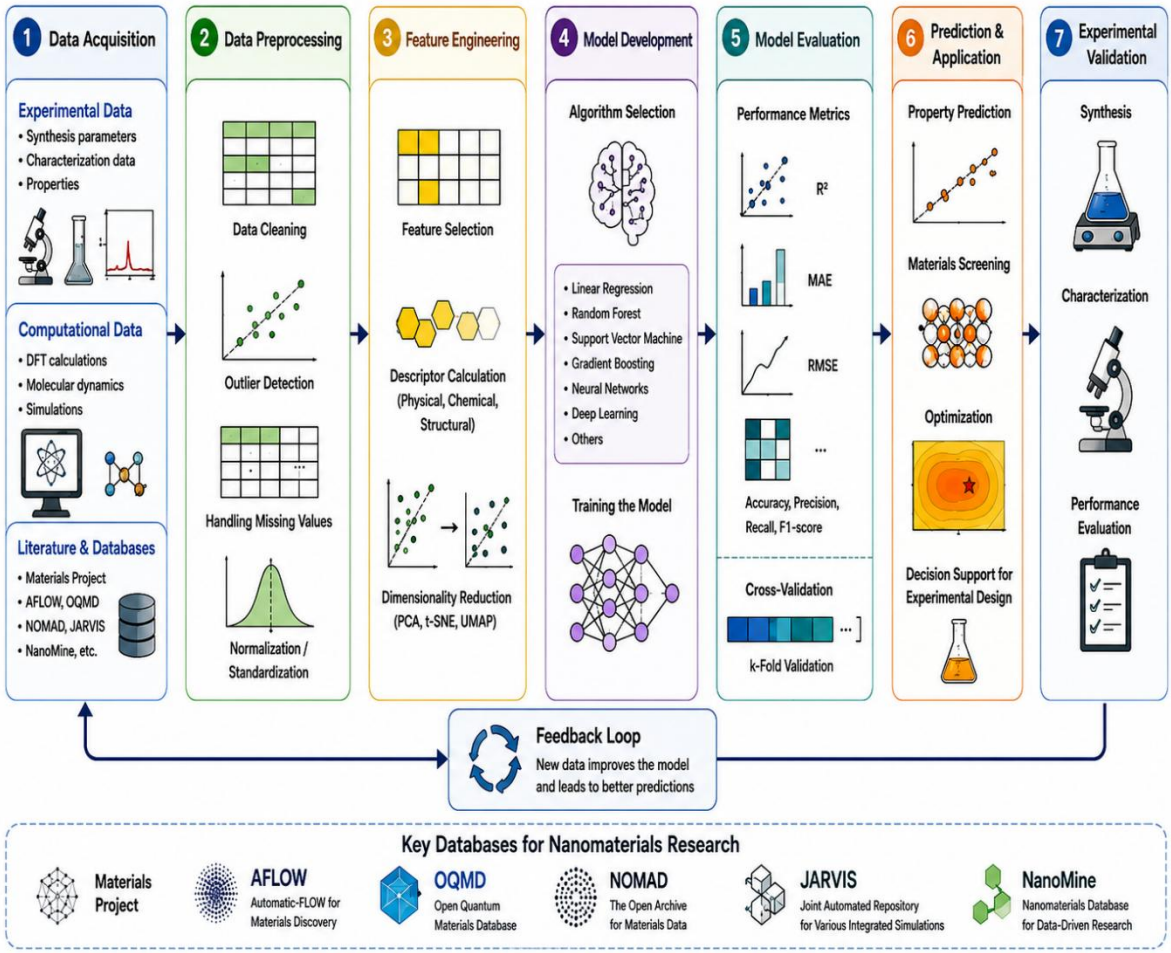

Fig. 1. General workflow of machine learning-based nanomaterials research from data acquisition to experimental validation and continuous model improvement.

3 | Machine Learning for Nanomaterial Discovery and Design

The discovery and design of advanced nanomaterials have traditionally relied on iterative experimental investigations and computational simulations, which are often time-consuming, resource-intensive, and limited by the vastness of the materials design space. Recent advances in ML have fundamentally transformed this process by enabling data-driven exploration of complex materials systems, accelerating property prediction, optimizing synthesis conditions, and identifying promising nanomaterial candidates with significantly reduced experimental effort. This section reviews the key ML strategies that are reshaping nanomaterial discovery and design, including accelerated materials screening, property prediction, synthesis optimization, and emerging AI-driven approaches such as High-Throughput Screening (HTS) and generative AI [30].

3.1 | Accelerating the Discovery of Novel Nanomaterials

The discovery of advanced nanomaterials has traditionally relied on experimental trial-and-error approaches and computational simulations, both of which require considerable time and resources. The enormous design space associated with nanomaterials including variations in chemical composition, crystal structure, morphology, particle size, surface functionalization, and synthesis conditions makes the identification of optimal materials a complex and labor-intensive process. Consequently, there is a growing demand for intelligent computational strategies capable of accelerating materials discovery while reducing experimental costs [31].

ML has emerged as a powerful tool for exploring multidimensional materials spaces by learning complex relationships between material descriptors and functional properties from existing datasets. Unlike conventional computational approaches that often require solving complex physical equations, ML models rapidly identify hidden correlations and predict the performance of unexplored nanomaterials. This capability enables researchers to screen thousands or even millions of candidate materials in a fraction of the time required for experimental investigations or high-fidelity simulations.

Recent studies have demonstrated that supervised learning algorithms, including RF, GB, SVM, and ANNs, can accurately predict key material properties such as thermal conductivity, electrical conductivity, band gap, adsorption capacity, catalytic activity, and mechanical strength. These predictive capabilities significantly reduce the number of experimental trials by identifying the most promising material candidates before laboratory synthesis [30].

Beyond property prediction, ML has also facilitated the inverse design of nanomaterials, in which researchers begin with a target property and use AI models to determine the material composition or structural characteristics required to achieve the desired performance. This data-driven strategy represents a major shift from conventional forward design approaches and has accelerated the development of high-performance nanomaterials for applications in energy storage, catalysis, sensing, environmental remediation, and advanced manufacturing [28].

The integration of ML with experimental data, computational simulations, materials databases, and scientific literature has established a comprehensive framework for accelerating nanomaterial discovery and design. By combining multiple data sources with intelligent predictive models, ML enables efficient materials screening, property prediction, synthesis optimization, and experimental validation within a continuous feedback loop. The overall AI-driven framework for nanomaterial discovery and design is schematically illustrated in *Fig. 2*.

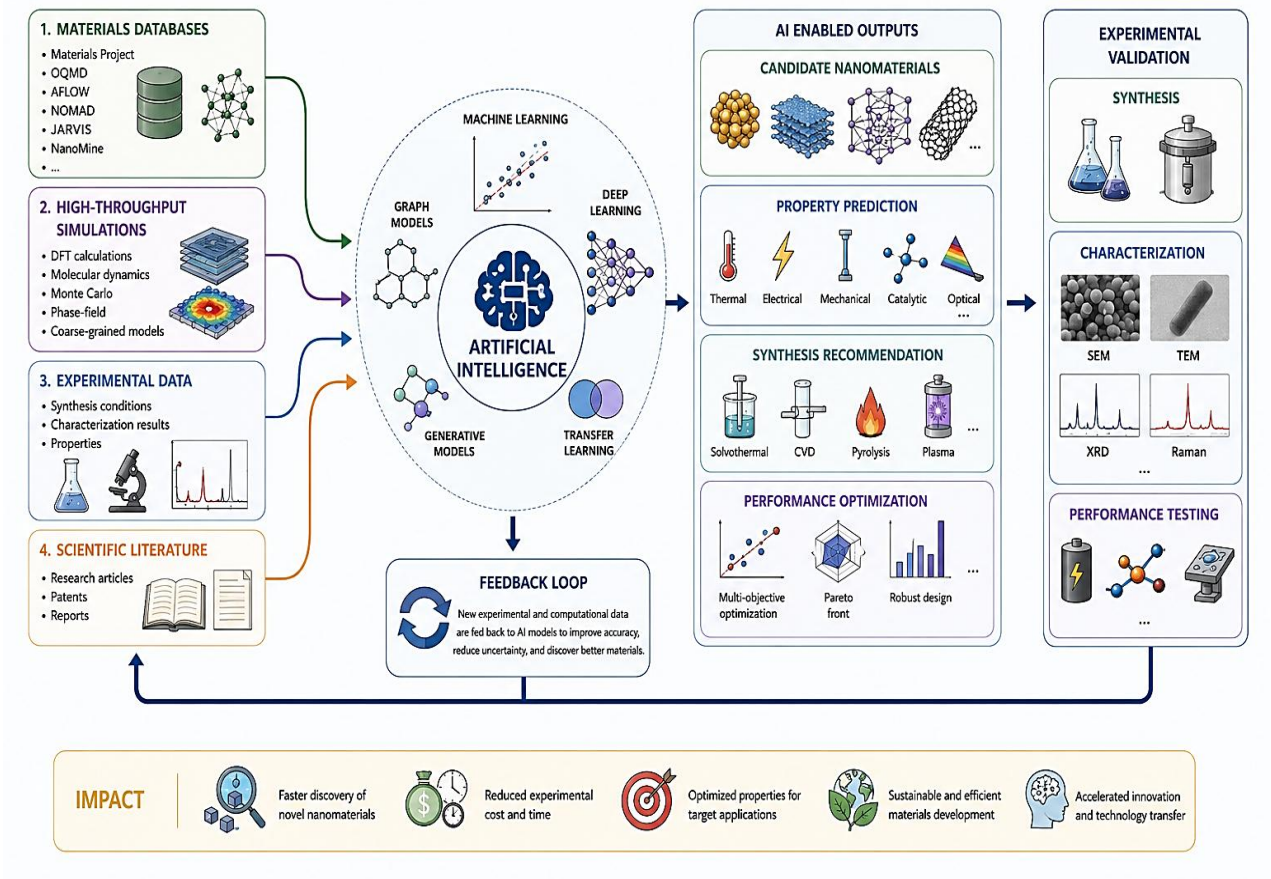

Fig. 2. Conceptual framework of AI-driven nanomaterial discovery and design using machine learning.

3.2 | Property Prediction and Performance Optimization of Nanomaterials

The accurate prediction of material properties is one of the most significant applications of ML in nanomaterials research. The physicochemical performance of nanomaterials is governed by numerous interconnected factors, including chemical composition, crystal structure, particle size, morphology, surface chemistry, synthesis conditions, and defect distribution. These complex and highly nonlinear relationships often limit the effectiveness of conventional theoretical models and empirical approaches. ML provides an efficient alternative by learning these relationships directly from experimental observations and computational datasets, enabling rapid prediction of material performance without exhaustive laboratory investigations [31].

Among the various applications of ML, the prediction of thermal, mechanical, electrical, optical, catalytic, and adsorption properties has received considerable attention. By utilizing descriptors extracted from experimental measurements, computational simulations, or materials databases, ML models can accurately estimate target properties and significantly reduce the time and cost associated with conventional trial-and-error experimentation. This capability has accelerated the development of high-performance nanomaterials for applications in energy conversion, environmental remediation, electronics, sensing, and advanced manufacturing. Supervised learning algorithms remain the dominant techniques for property prediction due to the availability of labeled datasets containing input descriptors and corresponding material properties. Algorithms such as RF, SVM, Extreme Gradient Boosting (XGBoost), ANNs, and GNNs have demonstrated excellent predictive performance across a wide range of nanomaterial systems. Ensemble learning methods, particularly RF and XGBoost, are widely employed because of their robustness against overfitting and their ability to capture nonlinear interactions among material descriptors. More recently, GNNs have attracted increasing interest because they directly represent atomic structures as graphs, allowing the prediction of material properties without extensive manual feature engineering. Thermal property prediction represents one of the most active research areas in AI-assisted nanomaterials development. ML models have been successfully applied to estimate thermal conductivity, heat capacity, thermal diffusivity, and interfacial thermal resistance in nanofluids, polymer nanocomposites, carbon-based nanomaterials, and ceramic nanostructures. Accurate prediction of these parameters enables researchers to identify promising thermal management materials before experimental synthesis, thereby considerably shortening the material development cycle [30].

Similarly, ML has demonstrated remarkable capability in predicting the mechanical behavior of nanomaterials, including tensile strength, elastic modulus, fracture toughness, hardness, and wear resistance. The integration of structural descriptors with advanced learning algorithms allows accurate estimation of mechanical performance under various loading conditions, supporting the design of lightweight and high-strength nanocomposites for structural and industrial applications.

Beyond thermal and mechanical characteristics, ML has become increasingly important for predicting electrical conductivity, band gap, optical absorption, photoluminescence, magnetic behavior, catalytic activity, and adsorption efficiency. These predictive capabilities have significantly accelerated the optimization of nanomaterials employed in batteries, supercapacitors, photocatalysts, gas sensors, water purification systems, and environmental monitoring technologies. The combination of predictive modeling with high-throughput computational screening further enables rapid identification of candidate materials exhibiting desired multifunctional properties [28–31]. As summarized in *Table 2*, different ML algorithms have demonstrated remarkable capabilities in predicting a wide range of nanomaterial properties, including thermal, mechanical, electrical, optical, catalytic, and adsorption characteristics, thereby accelerating materials optimization across diverse engineering applications.

ML has transformed property prediction from a computationally intensive and experimentally demanding process into a rapid data-driven framework capable of guiding materials design and optimization. As increasingly large and diverse datasets become available, AI-driven predictive models are expected to achieve higher accuracy, improved generalization, and greater applicability across a broad spectrum of functional nanomaterials [32].

Table 2. Representative machine learning applications for predicting nanomaterial properties.

Property	Representative Nanomaterials	Common ML Algorithms	Typical Applications
Thermal conductivity	Nanofluids, polymer nanocomposites	RF, XGBoost, ANN	Thermal management
Mechanical properties	Graphene, CNT composites	ANN, RF	Structural materials
Electrical conductivity	MXenes, graphene, metal oxides	GNN, ANN	Electronics and sensors
Optical properties	Quantum dots, plasmonic nanoparticles	CNN, RF	Photonics and imaging
Catalytic activity	MOFs, metal nanoparticles	GNN, XGBoost	Catalysis
Adsorption capacity	Nanocomposites, MOFs	RF, SVM	Water purification

3.3 | Machine Learning for Nanomaterial Synthesis Optimization

The synthesis of nanomaterials is a highly complex process involving numerous interconnected parameters, including precursor concentration, reaction temperature, pH, synthesis duration, solvent composition, pressure, mixing conditions, and post-treatment procedures. Small variations in these parameters can significantly influence particle size, morphology, crystallinity, surface chemistry, and ultimately the functional performance of the synthesized nanomaterials. Traditionally, optimization of synthesis conditions has relied on extensive experimental trial-and-error procedures, which are often labor-intensive, time-consuming, and economically inefficient. Consequently, ML has emerged as an effective computational strategy for optimizing nanomaterial synthesis by identifying complex nonlinear relationships between synthesis parameters and material characteristics.

Unlike conventional statistical optimization techniques, ML algorithms can simultaneously analyze multiple synthesis variables and capture intricate interactions that are difficult to identify using classical methods. Supervised learning models, including RF, SVM, ANNs, and XGBoost, have been widely employed to predict the influence of synthesis conditions on nanomaterial characteristics such as particle size distribution, crystallinity, specific surface area, porosity, and phase composition. These predictive models enable researchers to estimate the outcome of synthesis processes before conducting laboratory experiments, thereby substantially reducing experimental costs and development time.

ML has also facilitated intelligent process optimization through the integration of optimization algorithms such as Bayesian Optimization (BO), genetic algorithms, particle swarm optimization, and RL. These approaches continuously search the multidimensional design space to identify synthesis conditions that maximize specific target properties while minimizing resource consumption. Compared with traditional design-of-experiment methodologies, AI-assisted optimization provides significantly faster convergence toward optimal processing conditions and enables the efficient exploration of complex synthesis pathways.

Recent advances have further combined ML with robotic laboratories and autonomous experimentation platforms, allowing synthesis conditions to be automatically adjusted based on real-time experimental feedback. In these closed-loop systems, experimental measurements are continuously incorporated into predictive models, enabling iterative improvement of synthesis protocols with minimal human intervention. Such autonomous laboratories represent an important step toward self-driving materials discovery, where AI guides both computational predictions and experimental execution.

Another emerging application involves green nanomaterial synthesis, where ML assists in reducing chemical consumption, reaction time, energy demand, and environmental impact. By optimizing reaction parameters and identifying environmentally friendly synthesis routes, AI contributes to the development of sustainable nanomanufacturing processes that align with the principles of green chemistry and circular economy. These capabilities are becoming increasingly important as large-scale industrial production of nanomaterials continues to expand.

Overall, ML is transforming nanomaterial synthesis from an empirical and experience-based process into a predictive, data-driven, and highly automated methodology. The combination of intelligent optimization algorithms, autonomous experimentation, and sustainable manufacturing strategies is expected to play a central role in the future development of advanced nanomaterials for industrial and technological applications.

3.4 | High-Throughput Screening, Inverse Design, and Generative AI

Recent advances in AI have significantly expanded the role of ML beyond conventional property prediction toward autonomous materials discovery. HTS, inverse design, and Generative Artificial Intelligence (Generative AI) have emerged as transformative approaches for accelerating the development of advanced nanomaterials. These techniques enable researchers to efficiently explore vast design spaces while minimizing experimental effort and computational cost [33].

HTS combines computational simulations, experimental databases, and ML algorithms to rapidly evaluate thousands or even millions of potential nanomaterial candidates. Instead of experimentally synthesizing every possible material, predictive models estimate key performance indicators and rank candidate materials according to predefined objectives. This significantly shortens the discovery cycle while improving the efficiency of materials selection [28].

Inverse design represents a paradigm shift in nanomaterials research. Unlike conventional forward design, where material properties are evaluated after synthesis, inverse design begins with predefined target properties and employs AI algorithms to identify material compositions, structural characteristics, or processing conditions capable of achieving the desired performance. This approach has demonstrated considerable potential for designing nanomaterials with optimized thermal, electrical, catalytic, and mechanical properties. More recently, generative AI has emerged as a promising tool for creating entirely new nanomaterial candidates. Deep generative models, including Variational Autoencoders (VAEs), Generative Adversarial Networks (GANs), and diffusion models, are capable of learning complex materials distributions and generating novel structures that satisfy specific design constraints. These approaches substantially expand the searchable design space and facilitate the discovery of previously unexplored nanomaterials with tailored functionalities. The integration of HTS, inverse design, and generative AI is expected to establish autonomous materials discovery platforms in which computational prediction, intelligent optimization, and experimental validation operate within a continuous feedback loop. Such AI-driven frameworks have the potential to revolutionize nanomaterials research by reducing development time, lowering research costs, and accelerating the transition from computational discovery to practical implementation [34].

4 | Machine Learning Applications in Nanomaterials

The rapid advancement of ML has significantly expanded its applications across diverse areas of nanomaterials research, extending beyond materials discovery to encompass characterization, performance optimization, manufacturing, and industrial implementation. By integrating AI with advanced experimental techniques, computational modeling, and high-throughput data analysis, ML has enabled faster, more accurate, and cost-effective solutions for complex nanotechnology challenges [29–31]. This section reviews the major application domains of ML in nanomaterials, including intelligent characterization, energy and environmental technologies, nanoelectronics, smart sensing, and advanced manufacturing, highlighting how AI-driven methodologies are transforming both fundamental research and practical applications.

4.1 | Machine Learning for Nanomaterial Characterization

Nanomaterial characterization is a critical step in understanding the structural, morphological, chemical, and functional properties of nanoscale materials. Conventional characterization techniques, including SEM, TEM, AFM, XRD, Raman spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), and XPS, generate large volumes of complex experimental data that often require extensive interpretation by experienced researchers. The increasing complexity of nanomaterial systems has created a growing demand for intelligent analytical

tools capable of extracting meaningful information from these datasets with higher speed and accuracy. ML has emerged as an efficient approach for automated analysis of characterization data. Advanced algorithms can recognize hidden patterns, classify material structures, identify defects, and quantify microstructural features directly from microscopy images and spectroscopic signals [31]. Compared with conventional manual interpretation, AI-assisted analysis significantly reduces human bias while improving reproducibility and analytical efficiency. DL techniques, particularly CNNs, have demonstrated exceptional performance in processing microscopy images. CNN-based models can automatically identify nanoparticles, grain boundaries, crystal defects, pores, and surface irregularities from SEM and TEM images without requiring extensive manual feature extraction. Similarly, ML algorithms have been successfully applied to analyze diffraction patterns and spectroscopic data, enabling rapid phase identification, crystal structure classification, chemical composition analysis, and defect detection [35].

Recent developments have further integrated AI with automated microscopy systems, allowing real-time image acquisition and intelligent analysis during experimental characterization. Such AI-assisted characterization platforms reduce data processing time while improving measurement accuracy and consistency. As characterization datasets continue to expand, ML is expected to become an indispensable component of next-generation nanomaterials research by enabling faster, more reliable, and highly automated materials analysis.

4.2 | Machine Learning in Energy-Related Nanomaterials

ML has become an indispensable tool for accelerating the development of nanomaterials used in energy conversion and storage systems. AI-driven predictive models enable researchers to rapidly identify promising materials with enhanced electrochemical, thermal, and electronic properties while significantly reducing experimental costs and computational time. The integration of ML with computational materials science has accelerated the discovery of next-generation nanomaterials for sustainable energy technologies.

In battery research, ML has been widely applied to predict electrode performance, cycling stability, ionic conductivity, and energy density of lithium-ion, sodium-ion, and solid-state battery materials. Similarly, AI-assisted optimization has improved the design of nanostructured supercapacitors by identifying optimal electrode compositions and pore architectures for enhanced charge storage [33].

ML has also demonstrated remarkable potential in photovoltaic materials, hydrogen storage systems, thermoelectric materials, and fuel-cell catalysts. By combining high-throughput simulations with predictive algorithms, researchers can efficiently screen thousands of candidate nanomaterials and identify those exhibiting superior energy conversion efficiency and long-term stability. Consequently, AI-driven energy materials research is expected to play a key role in achieving future sustainable energy solutions.

4.3 | Machine Learning for Environmental Nanotechnology

Environmental nanotechnology has greatly benefited from recent advances in ML. AI techniques facilitate the design and optimization of nanomaterials for pollutant removal, water purification, air filtration, photocatalysis, and environmental monitoring. Predictive models enable researchers to evaluate adsorption capacity, catalytic efficiency, and degradation performance without relying solely on extensive laboratory experiments. ML has been successfully applied to optimize nanomaterials used for heavy metal adsorption, organic dye removal, pharmaceutical contaminant degradation, and carbon dioxide capture. Advanced algorithms identify relationships between structural descriptors and environmental performance, thereby accelerating the development of highly efficient remediation materials [34]. Furthermore, AI-assisted environmental monitoring systems integrate nanosensors with intelligent data analysis to enable rapid detection of pollutants and hazardous compounds. These developments contribute to more sustainable environmental protection strategies while reducing operational costs and improving decision-making processes.

4.4 | Machine Learning in Nanoelectronics and Smart Sensors

AI is transforming the design and optimization of nanoelectronic devices and intelligent sensing systems. ML algorithms support the development of high-performance nanomaterials for transistors, flexible electronics, wearable devices, gas sensors, biosensors, and quantum technologies by accurately predicting electrical and electronic properties.

DL techniques are increasingly employed for signal processing, pattern recognition, and sensor calibration, improving the sensitivity, selectivity, and stability of nanosensors. In addition, GNNs and other advanced learning models facilitate the discovery of novel two-dimensional materials, conductive nanocomposites, and semiconductor nanostructures suitable for next-generation electronic applications. The combination of ML with nanoelectronics enables intelligent sensing platforms capable of real-time monitoring, autonomous decision-making, and adaptive system optimization, thereby supporting the development of smart healthcare, environmental monitoring, and industrial automation technologies [33–35].

4.5 | Industrial Manufacturing and Process Optimization

ML has become a driving force in the digital transformation of nanomaterial manufacturing. AI-based models optimize synthesis conditions, monitor production processes, predict product quality, and improve manufacturing efficiency through intelligent process control and predictive analytics. Modern industrial facilities increasingly employ ML for quality inspection, defect detection, predictive maintenance, process monitoring, and digital twin technologies. These intelligent manufacturing systems minimize material waste, reduce production costs, and enhance process reliability while maintaining consistent product quality. The integration of ML with Industry 4.0 and emerging Industry 5.0 technologies is expected to further automate nanomaterial production by enabling autonomous manufacturing systems capable of continuous learning, self-optimization, and real-time process adaptation [36].

Fig. 3 provides a schematic overview of the major application domains of ML in nanotechnology, whereas representative nanomaterials, commonly employed ML algorithms, and their typical outcomes are comprehensively summarized in *Table 3*.

Table 3. Representative applications of machine learning across major nanotechnology sectors.

Application Area	Representative Nanomaterials	Typical Machine Learning Tasks	Common AI/ML Algorithms	Representative Outcomes
Nanomaterial characterization	Nanoparticles, CNTs, Graphene, MXenes	Image classification, phase identification, defect detection, spectral analysis	CNN, Vision Transformer (ViT), RF, SVM	Automated characterization, defect recognition, improved analytical accuracy
Energy nanotechnology	Battery electrodes, Perovskites, MXenes, Nanocomposites	Property prediction, materials screening, lifetime estimation, performance optimization	ANN, GNN, XGBoost, BO	Enhanced batteries, supercapacitors, solar cells, hydrogen storage systems
Environmental nanotechnology	MOFs, Metal oxides, Carbon nanomaterials, Polymer nanocomposites	Adsorption prediction, photocatalytic optimization, pollutant classification	RF, XGBoost, ANN, SVM	Water purification, air remediation, pollutant degradation, environmental monitoring
Nanoelectronics & smart sensors	Graphene, Quantum dots, 2D materials, Conductive polymers	Conductivity prediction, signal processing, sensor optimization	GNN, CNN, ANN, DL	High-performance sensors, wearable electronics, flexible devices, intelligent sensing

Table 3. Continued.

Application Area	Representative Nanomaterials	Typical Machine Learning Tasks	Common AI/ML Algorithms	Representative Outcomes
Industrial manufacturing	Ceramic nanomaterials, Polymer nanocomposites, Functional coatings	Process optimization, quality control, predictive maintenance, defect detection	RL, DL, RF	Smart manufacturing, automated production, digital twins, reduced production cost
Healthcare & biomedical (emerging)	Nano-biosensors, Diagnostic nanoparticles	Pattern recognition, image analysis, biosignal classification	CNN, Transformer models	Intelligent diagnostics, rapid biosensing (included for completeness, although not emphasized in this review)

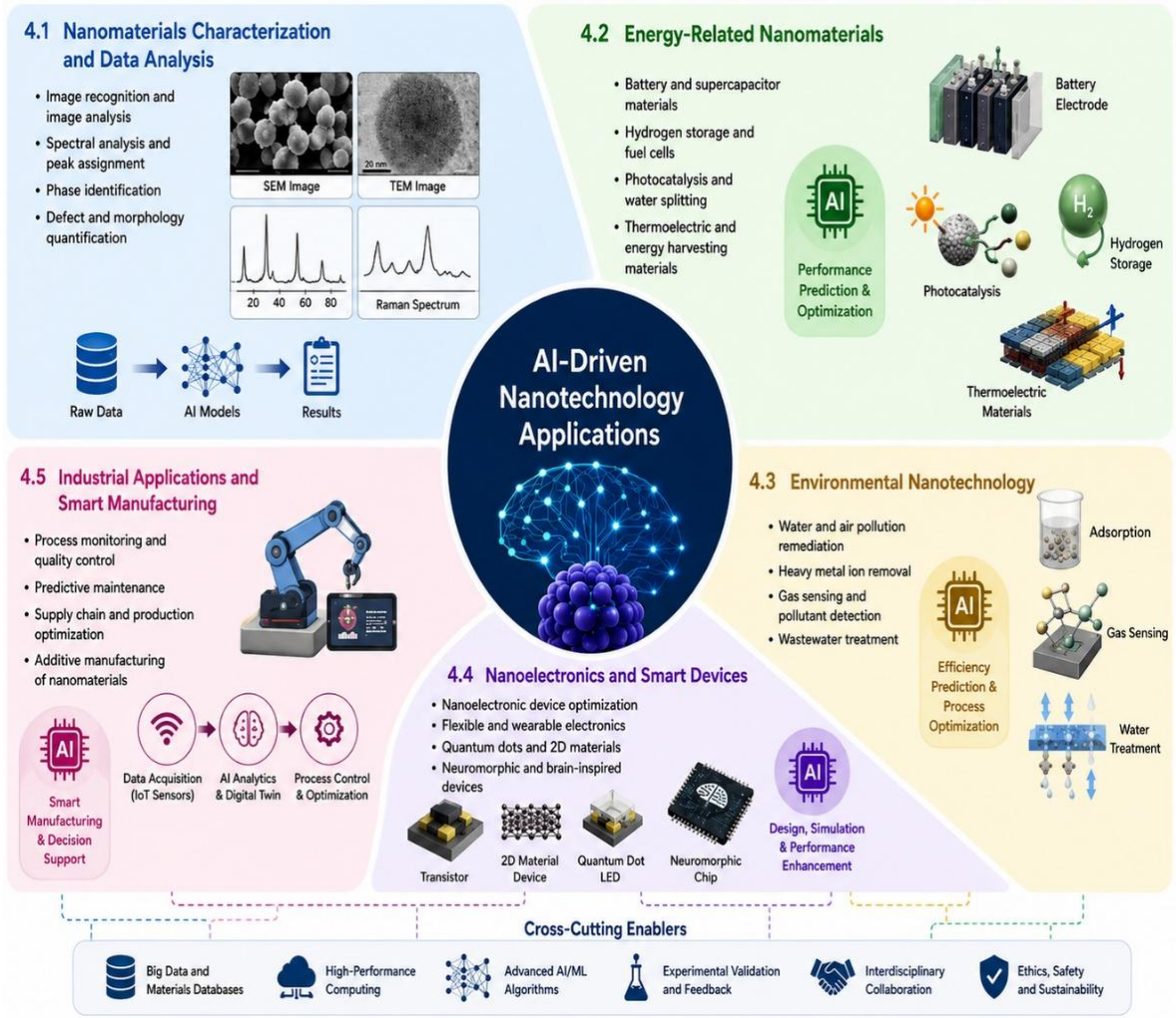

Fig. 3. Schematic overview of machine learning applications in nanotechnology.

5|Emerging Trends and Future Opportunities in AI-Driven Nanomaterials Research

The continuous evolution of AI is expected to redefine the future landscape of nanomaterials research by enabling more autonomous, predictive, and intelligent approaches for materials discovery and development. While conventional ML methods have already demonstrated significant capabilities in property prediction,

synthesis optimization, and characterization analysis, emerging AI technologies are extending these capabilities toward more comprehensive and self-improving materials development frameworks. The future of nanotechnology is expected to be increasingly driven by the integration of advanced AI models, large-scale materials data, autonomous experimentation, and digital engineering platforms [34].

5.1 | Explainable Artificial Intelligence for Nanomaterials

Although ML models have achieved remarkable predictive accuracy, their practical adoption in nanomaterials research is often limited by insufficient interpretability. XAI has emerged as a promising approach to overcome this limitation by providing insights into the relationships between input descriptors, structural features, processing parameters, and predicted material properties. Unlike conventional black-box models, explainable AI methods can identify the most influential factors controlling material performance and provide physically meaningful interpretations of model predictions [30–32]. The integration of XAI with nanomaterials research can significantly improve the reliability of AI-assisted decision-making by enabling researchers to understand why specific materials exhibit superior properties. For example, explainable models can reveal the contribution of particle size, surface chemistry, crystal structure, or compositional features to catalytic activity, conductivity, adsorption capacity, or mechanical performance. Such knowledge not only improves model confidence but also facilitates the development of new materials based on scientific understanding rather than purely computational predictions.

5.2 | Foundation Models and Large-Scale Materials Intelligence

Recent advances in foundation models represent a major transformation in AI, allowing models to learn complex patterns from large and diverse datasets. Similar to large-scale AI models developed in other scientific fields, materials foundation models have the potential to integrate information from experimental measurements, computational simulations, scientific literature, and material databases to provide comprehensive predictions across multiple property domains [37].

In nanomaterials research, foundation models may enable transfer learning approaches, where knowledge obtained from existing materials systems can be transferred to new and unexplored nanomaterial classes. This capability is particularly valuable for addressing the challenge of limited experimental datasets, as models can achieve improved performance by learning general relationships between composition, structure, processing conditions, and functionality. Future development of large-scale materials intelligence platforms may significantly accelerate the discovery of multifunctional nanomaterials with tailored properties.

5.3 | Autonomous Laboratories and Self-Driving Materials Discovery

One of the most promising future directions in nanomaterials research is the emergence of autonomous laboratories that combine AI, robotics, and advanced characterization techniques. In these systems, ML algorithms can design experiments, determine optimal synthesis conditions, analyze experimental results, and iteratively improve predictions through closed-loop feedback. Self-driving laboratories have the potential to dramatically reduce experimental time and resources by replacing conventional sequential experimentation with intelligent autonomous optimization. Such platforms can continuously explore complex synthesis spaces, identify optimal processing conditions, and accelerate the development of nanomaterials for applications in energy, environmental technologies, electronics, and advanced manufacturing [38].

5.4 | Digital Twins and Sustainable Nanomanufacturing

Digital twin technology represents another emerging opportunity for integrating AI with nanomaterials engineering. A digital twin is a virtual representation of a physical process or material system that continuously incorporates real-time data to simulate, monitor, and optimize performance. In nanomanufacturing, digital twins can enable predictive process control, quality optimization, and efficient resource management.

The combination of digital twins with ML can support sustainable nanomaterial production by reducing energy consumption, minimizing material waste, and improving process reliability. These intelligent manufacturing approaches are particularly important for the transition of nanomaterials from laboratory-scale development toward large-scale industrial production [30–34].

5.5 | Multimodal Artificial Intelligence for Comprehensive Nanomaterials Understanding

Future advances in AI-driven nanomaterials research will increasingly depend on the integration of multimodal data sources. Nanomaterials generate diverse datasets, including microscopy images, spectroscopic signals, structural information, computational simulations, and experimental performance measurements. Conventional ML models often analyze these data types independently, limiting their ability to capture the complete relationship between material structure and functionality. Multimodal AI approaches aim to combine different data representations within unified learning frameworks, enabling more accurate and comprehensive understanding of nanomaterial behavior. By integrating visual, chemical, structural, and performance-related information, multimodal AI models can provide deeper insights into materials systems and support more reliable predictions for complex [37]. The emerging AI technologies and their potential contributions to future nanomaterials research are summarized in *Table 4*.

Table 4. Emerging AI-driven technologies and future opportunities in nanomaterials research.

Emerging Trend	Current Role in Nanomaterials Research	Potential Applications	Future Opportunities
Explainable artificial intelligence	Improves interpretation of ML predictions and identifies important material descriptors	Understanding structure–property relationships, catalyst design, property prediction	Development of transparent and trustworthy AI models for scientific discovery
Foundation models for materials science	Enables learning from large-scale experimental, computational, and literature-based datasets	Multi-property prediction, transfer learning, accelerated materials screening	Creation of universal AI models capable of predicting diverse nanomaterial behaviors
Generative artificial intelligence	Generates new material structures and compositions based on predefined targets	Inverse design of nanomaterials, optimization of functional properties	Autonomous generation of novel nanomaterials with tailored performance
Autonomous laboratories	Combines AI algorithms with robotics and automated experimentation	Automated synthesis, characterization, and optimization of nanomaterials	Closed-loop self-driving laboratories for accelerated materials discovery
Digital twin technology	Creates virtual representations of materials and manufacturing processes	Process monitoring, prediction, and optimization of nanomaterial production	Intelligent and sustainable nanomanufacturing systems
Multimodal AI approaches	Integrates diverse data sources including microscopy, spectroscopy, simulations, and experiments	Comprehensive materials understanding and improved prediction accuracy	Development of unified AI platforms for complex nanomaterial systems
Graph neural networks	Represents atomic structures and material interactions as graph-based data	Crystal structure prediction, molecular representation, property estimation	Advanced modeling of complex nanoscale structures and interactions
Physics-Informed Machine Learning (PIML)	Incorporates physical laws and scientific knowledge into AI models	More reliable prediction with limited experimental data	Hybrid AI–physics frameworks for accurate and interpretable nanomaterials modeling
AI-enabled sustainable nanotechnology	Uses AI to optimize resource utilization and environmental performance	Green synthesis, energy-efficient production, lifecycle optimization	Development of sustainable and environmentally responsible nanomaterials

6 | Challenges, Limitations, and Future Perspectives

Despite the remarkable progress achieved in integrating ML with nanomaterials research, several scientific and technical challenges remain to be addressed before AI-driven methodologies can be fully adopted in both academic research and industrial practice. Although ML has significantly accelerated materials discovery, property prediction, synthesis optimization, and intelligent characterization, its predictive performance strongly depends on the availability of high-quality datasets, appropriate feature representation, and robust model generalization. One of the primary challenges is the limited availability of standardized and comprehensive nanomaterial datasets. Experimental data are often generated using different synthesis protocols, characterization techniques, and reporting standards, leading to inconsistencies that reduce model reliability and reproducibility. Furthermore, many publicly available datasets remain relatively small compared with those used in other AI applications, restricting the performance of data-intensive DL models [32–38].

Another important limitation concerns the interpretability of ML models. While deep neural networks frequently achieve high predictive accuracy, they are commonly regarded as "black-box" models, providing limited insight into the underlying physical mechanisms governing material behavior. Consequently, increasing attention has been devoted to XAI, which aims to improve model transparency and enhance researchers' confidence in AI-assisted decision-making. Model transferability also remains a significant challenge. Many predictive models perform well only within the specific materials systems used during training and exhibit reduced accuracy when applied to new material classes or different experimental conditions [35]. Developing generalized ML frameworks capable of accurately predicting diverse nanomaterial systems remains an active area of research. Looking toward the future, the integration of ML with autonomous laboratories, robotic experimentation, digital twins, and high-throughput characterization platforms is expected to fundamentally transform nanomaterials research. These intelligent systems will enable closed-loop materials discovery, where AI continuously designs experiments, predicts material performance, analyzes characterization results, and optimizes synthesis conditions with minimal human intervention. Recent advances in foundation models, GNNs, large language models, and generative AI are expected to further expand the capabilities of AI-assisted nanomaterials research. These technologies will facilitate the discovery of previously unexplored materials, improve predictive accuracy across multiple property domains, and accelerate the transition from computational design to industrial implementation [34–38]. Future progress will largely depend on interdisciplinary collaboration among materials scientists, chemists, physicists, computer scientists, and data engineers to establish standardized databases, transparent AI models, and reliable validation protocols for next-generation intelligent materials research. The major challenges limiting the widespread application of ML in nanomaterials research, along with potential strategies and future opportunities, are summarized in *Table 5*.

Table 5. Major challenges, current limitations, and future opportunities in AI-driven nanomaterials research.

Challenge/Limitation	Current Situation in Nanomaterials Research	Impact on Machine Learning Performance	Potential Solutions and Future Opportunities
Limited availability of high-quality datasets	Experimental nanomaterials data are often limited, heterogeneous, and generated under different synthesis and characterization conditions	Reduces model accuracy, reliability, and generalization capability	Development of standardized open-access materials databases, data-sharing platforms, and large-scale collaborative datasets
Data inconsistency and lack of standardization	Different laboratories frequently use different reporting formats, measurement protocols, and characterization methods	Creates uncertainty and decreases reproducibility of AI predictions	Establishment of unified data formats, standardized experimental protocols, and FAIR (Findable, Accessible, Interoperable, Reusable) data principles

Table 5. Continued.

Challenge/Limitation	Current Situation in Nanomaterials Research	Impact on Machine Learning Performance	Potential Solutions and Future Opportunities
Limited model interpretability	Many advanced deep learning models operate as black-box systems with limited physical explanation	Reduces researchers' confidence and limits scientific understanding of predicted relationships	Integration of Explainable AI (XAI), feature importance analysis, and physics-informed machine learning approaches
Poor generalization across different nanomaterial systems	Models trained on specific materials often perform poorly when applied to new material classes or unexplored compositions	Restricts practical application and transferability of predictive models	Development of transfer learning, foundation models, graph neural networks, and multi-task learning frameworks
Insufficient integration between computational and experimental approaches	Many AI models are developed independently from experimental validation processes	Limits practical applicability and slows materials development cycles	Integration of machine learning with autonomous laboratories, robotic synthesis, and closed-loop experimental platforms
Complex relationship between structure, processing, and properties	Nanomaterial performance depends on multiple interacting parameters including composition, morphology, defects, and processing conditions	Makes accurate prediction challenging using conventional ML approaches	Use of multimodal AI models combining microscopy, spectroscopy, simulation, and experimental datasets
High computational requirements	Advanced deep learning models and large-scale simulations require significant computational resources	Increases development time and limits accessibility for researchers	Utilization of cloud computing, efficient algorithms, model compression, and high-performance computing platforms
Lack of industrial-scale implementation	Many AI-assisted nanomaterials approaches remain at laboratory research stages	Creates a gap between academic discoveries and commercial applications	Integration of AI with Industry 4.0/5.0, digital twins, smart manufacturing, and real-time process monitoring
Ethical and reliability concerns	AI-generated predictions require careful validation before practical implementation	Incorrect predictions may lead to inefficient material development or unreliable decisions	Establishment of validation frameworks, uncertainty quantification, and responsible AI practices
Sustainability considerations	AI models often focus on performance improvement without fully considering environmental impacts	May overlook energy consumption, resource efficiency, and lifecycle impacts	Development of sustainable AI-driven materials design considering green synthesis and life-cycle assessment

7 | Conclusion

The rapid convergence of nanotechnology and AI has established ML as one of the most transformative technologies in modern materials science. By enabling data-driven analysis of complex material systems, ML has significantly accelerated the discovery, design, characterization, and optimization of nanomaterials while reducing the dependence on traditional trial-and-error experimentation [21]. This review comprehensively summarized the recent advances in ML applications across the entire nanomaterial development pipeline, highlighting its growing role in intelligent materials engineering. The review first discussed the fundamental concepts of ML and their relevance to nanomaterials research, emphasizing the characteristics of supervised, unsupervised, reinforcement, and DL approaches. The integration of computational modeling, experimental data, and materials databases has created an efficient framework for AI-assisted nanomaterial research,

allowing predictive models to identify hidden relationships among structural descriptors, synthesis parameters, and functional properties. These developments have transformed conventional materials research into a predictive and data-driven discipline [21–24].

One of the most significant contributions of ML lies in nanomaterial discovery and design. Advanced algorithms have enabled rapid screening of enormous materials spaces, accurate prediction of physicochemical properties, and optimization of synthesis conditions with considerably reduced experimental effort. Recent developments in inverse design, HTS, and generative AI have further expanded the capabilities of AI by enabling the creation of entirely new nanomaterial candidates that satisfy predefined performance requirements. These approaches are expected to substantially shorten the time required for developing advanced functional nanomaterials while reducing research costs and improving design efficiency [23].

The review also highlighted the broad applications of ML across diverse nanotechnology sectors. Intelligent algorithms have demonstrated remarkable performance in automated nanomaterial characterization through microscopy and spectroscopy analysis, enabling rapid defect detection, phase identification, and structural interpretation. Furthermore, ML has become an essential tool for developing nanomaterials for energy storage and conversion systems, environmental remediation technologies, nanoelectronics, smart sensors, and intelligent manufacturing. The combination of predictive modeling with autonomous optimization provides new opportunities for designing highly efficient materials tailored to specific engineering applications. Despite these remarkable achievements, several important challenges continue to limit the widespread implementation of ML in nanomaterials research [24]. The availability of high-quality, standardized, and sufficiently large datasets remains one of the major obstacles to developing robust predictive models. In addition, improving model interpretability, ensuring reliable generalization across different material systems, and establishing transparent validation protocols remain critical research priorities. Addressing these challenges will require stronger collaboration among materials scientists, chemists, physicists, computer scientists, and data engineers, together with the development of open-access databases and standardized reporting frameworks. Looking forward, the future of nanomaterials research is expected to be increasingly driven by intelligent, autonomous, and data-centric methodologies [20–28]. Emerging technologies such as XAI, GNNs, foundation models, generative AI, digital twins, autonomous laboratories, and robotic experimentation are expected to fundamentally reshape the way nanomaterials are discovered, synthesized, characterized, and manufactured. Rather than serving solely as predictive tools, future AI systems will increasingly function as intelligent research partners capable of continuously integrating computational predictions, experimental observations, and process optimization within closed-loop materials development platforms [26–28]. In conclusion, ML is no longer merely a complementary computational technique but has become a fundamental enabling technology for next-generation nanomaterials research. Its ability to accelerate materials discovery, optimize synthesis processes, predict functional properties, and support intelligent manufacturing positions AI at the forefront of future nanotechnology innovation. Continued advances in algorithms, data infrastructure, and interdisciplinary collaboration will further strengthen the integration of ML into nanoscience, paving the way toward faster, more sustainable, and highly autonomous development of advanced nanomaterials for scientific, industrial, and societal applications.

Authors' Contributions

All aspects of the research and manuscript preparation were carried out by the author. The author has read and approved the final version of the manuscript.

Data Availability

All data supporting the reported findings in this research paper are provided within the manuscript.

Funding

Not applicable.

Conflict of Interest

The author declares that they do not have any conflict of interest.

Consent for Publication

The author confirms consent for the publication of this work

Ethics Approval and Consent to Participate

This article does not contain any studies with human participants performed by the author.

References

[1] Malica, C., Novoselov, K. S., Barnard, A. S., Kalinin, S. V., Spurgeon, S. R., Reuter, K., ... & Roche, S. (2025). Artificial intelligence for advanced functional materials: Exploring current and future directions. *Journal of Physics: Materials*, *8*(2), 21001. https://doi.org/10.1088/2515-7639/adc29d

[2] Das, H., & Sharma, M. (2025). Transforming computational nanotechnology: Accelerating material discovery, design, and property prediction through soft computing techniques. *ACS Applied Electronic Materials*, *7*(13), 5757–5787. https://doi.org/10.1021/acsaelm.5c00842

[3] Zhou, H., Xu, J., Qin, X., Zhang, J., Zou, W., Shakouri, M., … & Pang, H. (2025). Machine learning-driven material intelligence research and development. *Nano Research*, *18*(12), 94908095. https://doi.org/10.26599/NR.2025.94908095

[4] del Bosque, A., Fernández-Arias, P., & Vergara, D. (2026). Machine learning for nanomaterial discovery and design. *Machine Learning and Knowledge Extraction*, *8*(1), 10. https://doi.org/10.3390/make8010010

[5] Goga, A. S. (2024). Integrating artificial intelligence in nanomaterials science: Pathways to revolutionary materials discovery and design. ethics and risks. *International Conference on Innovative Research* (pp. 1–11). Springer. https://doi.org/10.1007/978-3-031-81198-2_1

[6] Boretti, A. (2026). Artificial Intelligence-driven nanomaterials: Pioneering innovations in energy conversion and storage. *Expert Systems*, *43*(7), e70310. https://doi.org/10.1111/exsy.70310

[7] Mim, J. J., Rakib, S., Akter, S., Nisha, J. R., Khan, S., Rahman, S. M. M., … & Hossain, N. (2025). The emerging role of machine learning in nanomaterials research: Applications, challenges, and future directions. *Journal of Nanoparticle Research*, *27*(11), 282. https://doi.org/10.1007/s11051-025-06472-2

[8] Jia, Y., Hou, X., Wang, Z., & Hu, X. (2021). Machine learning boosts the design and discovery of nanomaterials. *ACS Sustainable Chemistry & Engineering*, *9*(18), 6130–6147. https://doi.org/10.1021/acssuschemeng.1c00483

[9] Konstantopoulos, G., Koumoulos, E. P., & Charitidis, C. A. (2022). Digital innovation enabled nanomaterial manufacturing; machine learning strategies and green perspectives. *Nanomaterials*, *12*(15), 2646. https://doi.org/10.3390/nano12152646

[10] Huang, G., Guo, Y., Chen, Y., & Nie, Z. (2023). Application of machine learning in material synthesis and property prediction. *Materials*, *16*(17), 5977. https://doi.org/10.3390/ma16175977

[11] Vasudevan, R., Pilania, G., & Balachandran, P. V. (2021). Machine learning for materials design and discovery. *Journal of Applied Physics*, *129*(7), 070401. https://doi.org/10.1063/5.0043300

[12] Cai, J., Chu, X., Xu, K., Li, H., & Wei, J. (2020). Machine learning-driven new material discovery. *Nanoscale Advances*, *2*(8), 3115–3130. https://doi.org/10.1039/d0na00388c

[13] Madika, B., Saha, A., Kang, C., Buyantogtokh, B., Agar, J., Wolverton, C. M., … & Hong, S. (2025). Artificial intelligence for materials discovery, development, and optimization. *ACS Nano*, *19*(30), 27116–27158. https://doi.org/10.1021/acsnano.5c04200

[14] Wang, H., Cao, H., & Yang, L. (2024). Machine learning-driven multidomain nanomaterial design: From bibliometric analysis to applications. *ACS Applied Nano Materials*, *7*(23), 26579–26600. https://doi.org/10.1021/acsanm.4c04940

[15] Batra, R., Song, L., & Ramprasad, R. (2021). Emerging materials intelligence ecosystems propelled by machine learning. *Nature Reviews Materials*, *6*(8), 655–678. https://ui.adsabs.harvard.edu/link_gateway/2021NatRM...6..655B/doi:10.1038/s41578-020-00255-y

[16] Kumar Yadav, A. (2026). Artificial intelligence in accelerating materials discovery: Opportunities and challenges. *ChemistrySelect*, *11*(7), e07191. https://doi.org/10.1002/slct.202507191

[17] Pattebahadur, K. L., & Desmukh, S. D. (2026). AI and machine learning in material discovery. In *Recent Advancements in Materials Science* (p. 15). Redshine Publication UK. https://books.google.com/books?hl=en&lr=&id=_7TcEQAAQBAJ&oi=fnd&pg=PA15&dq=info:GKcLJn7JiI0J:scholar.google.com&ots=yJIp2fmLtg&sig=TYQKBIHEkqPsRH9MYUEMVXDAEFA#v=onepage&q&f=false

[18] Das, M., Perez, T. C., Shetty, D., Hiremath, P., Naik, N., & Bhat, R. (2024). An overview on the role of artificial intelligence in modern advancements of material science. *ES General*, *5*, 1183. https://doi.org/10.30919/esg1183

[19] Zhu, X., Li, Y., & Gu, N. (2023). Application of artificial intelligence in the exploration and optimization of biomedical nanomaterials. *Nano Biomedicine & Engineering*, *15*(3), 342–353. https://doi.org/10.26599/NBE.2023.9290035

[20] Winkler, D. A. (2020). Role of artificial intelligence and machine learning in nanosafety. *Small*, *16*(36), 2001883. https://doi.org/10.1002/smll.202001883

[21] Mishra, R. K., Mishra, D., & Agarwal, R. (2024). An artificial intelligence-powered approach to material design. *Cutting-Edge Research in Chemical and Material Science*, *1*, 1–15. https://www.researchgate.net/profile/Rajesh-Mishra-26/publication/383463608_An_Artificial_Intelligence-Powered_Approach_to_Material_Design/links/66cedeb3f84dd1716c6e6dca/An-Artificial-Intelligence-Powered-Approach-to-Material-Design.pdf

[22] Singh, A. V., Rosenkranz, D., Ansari, M. H. D., Singh, R., Kanase, A., Singh, S. P., … & Luch, A. (2020). Artificial intelligence and machine learning empower advanced biomedical material design to toxicity prediction. *Advanced Intelligent Systems*, *2*(12), 2000084. https://doi.org/10.1002/aisy.202000084

[23] Sharma, R., Singla, L., & Singh, G. (2025). Nanomaterials in the AI era: Revolutionizing research, design, and applications. In *AI-Driven Technologies for Sustainable Engineering* (pp. 1–26). Bentham Science Publishers. https://doi.org/10.2174/9798898129421250101

[24] Oviedo, L. R., Oviedo, V. R., Martins, M. O., Fagan, S. B., & Da Silva, W. L. (2022). Nanoarchitectonics: The role of artificial intelligence in the design and application of nanoarchitectures. *Journal of Nanoparticle Research*, *24*(8), 157. https://doi.org/10.1007/s11051-022-05535-y

[25] Agrawal, A., Singh, J., Jain, A., Tiwari, A. K., Kushwah, A. S., & Verma, N. K. (2026). Intelligent methods for materials discovery and design. In *Applications of AI in Materials Science* (pp. 1–28). IGI Global Scientific Publishing. https://doi.org/10.4018/979-8-3373-6127-7.ch001

[26] Badini, S., Regondi, S., & Pugliese, R. (2023). Unleashing the power of artificial intelligence in materials design. *Materials*, *16*(17), 5927. https://doi.org/10.3390/ma16175927

[27] Ibn-Mohammed, T., Mustapha, K. B., Abdulkareem, M., Fuensanta, A. U., Pecunia, V., & Dancer, C. E. J. (2023). Toward artificial intelligence and machine learning-enabled frameworks for improved predictions of lifecycle environmental impacts of functional materials and devices: T. Ibn-Mohammed et al. *MRS Communications*, *13*(5), 795–811. https://doi.org/10.1557/s43579-023-00480-w

[28] Shahzad, K., Mardare, A. I., & Hassel, A. W. (2024). Accelerating materials discovery: Combinatorial synthesis, high-throughput characterization, and computational advances. *Science and Technology of Advanced Materials: Methods*, *4*(1), 2292486. https://doi.org/10.1080/27660400.2023.2292486

[29] Rao, A. S. M., Koyada Prathap, D. E., Kiran, C. S., & Niran, I. R. (2026). Application of machine learning in material science: Predicting properties and performance of advanced materials. *Advanced Engineering Sciences*, *58*(1), 2668–2682.

[30] Bajaj, S. H., Nesamani, S. L., Dharmalingam, G., Jeeva, R., & Niveditha, V. R. (2024). The artificial intelligence-based revolution in material science for advanced energy storage. In *Introduction to Functional Nanomaterials* (pp. 85–92). CRC Press.

https://www.taylorfrancis.com/chapters/edit/10.1201/9781003495437-9/artificial-intelligence-based-revolution-material-science-advanced-energy-storage-sonia-bajaj-leena-nesamani-ganesan-dharmalingam-jeeva-niveditha

[31] Diao, S., Wu, Q., Li, S., Xu, G., Ren, X., Tan, L., … & Meng, X. (2025). From synthesis to properties: Expanding the horizons of machine learning in nanomaterials research. *Materials Horizons*, *12*(12), 4133–4164. https://doi.org/10.1039/d4mh01909a

[32] Silveira, R. F., Lima, A. L., Gross, I. P., Gelfuso, G. M., Gratieri, T., & Cunha-Filho, M. (2024). The role of artificial intelligence and data science in nanoparticles development: A review. *Nanomedicine*, *19*(14), 1271–1283. https://doi.org/10.1080/17435889.2024.2359355

[33] Liang, X., Yu, S., Meng, B., Ju, Y., Wang, S., & Wang, Y. (2025). Machine-learning-guided design of nanostructured metal oxide photoanodes for photoelectrochemical water splitting: From material discovery to performance optimization. *Nanomaterials*, *15*(12), 948. https://doi.org/10.3390/nano15120948

[34] Bai, X., & Zhang, X. (2025). Artificial intelligence-powered materials science. *Nano-Micro Letters*, *17*(1), 135. https://doi.org/10.1007/s40820-024-01634-8

[35] Rawat, P., Chaudhary, S., Kumar, N., & Babber, K. (2026). Role of artificial intelligence and machine learning in rare earth-doped metal oxide nanoparticles. In *Rare Earth-Doped Metal Oxide Nanostructures: for Energy Harvesting and Environmental Sensing* (pp. 85–103). Springer. https://doi.org/10.1007/978-981-95-6192-6_5

[36] Zhou, T., Song, Z., & Sundmacher, K. (2019). Big data creates new opportunities for materials research: A review on methods and applications of machine learning for materials design. *Engineering*, *5*(6), 1017–1026. https://doi.org/10.1016/j.eng.2019.02.011

[37] Chávez-Angel, E., Eriksen, M. B., Castro-Alvarez, A., Garcia, J. H., Botifoll, M., Avalos-Ovando, O., … & Mugarza, A. (2025). Applied artificial intelligence in materials science and material design. *Advanced Intelligent Systems*, *7*(8), 2400986. https://doi.org/10.1002/aisy.202400986

[38] Shen, L., Zhou, J., Yang, T., Yang, M., & Feng, Y. P. (2022). High-throughput computational discovery and intelligent design of two-dimensional functional materials for various applications. *Accounts of Materials Research*, *3*(6), 572–583. https://doi.org/10.1021/accountsmr.1c00246