https://doi.org/10.71058/jodac.v10i01002

ISSN: 1672 - 6553

JOURNAL OF DYNAMICS AND CONTROL

VOLUME 10 ISSUE 01: P12-38

NANOTECHNOLOGY EMPOWERED BY ARTIFICIAL INTELLIGENCE: A STATE-OF-THE-ART REVIEW ON MATERIAL SYNTHESIS AND CHARACTERIZATION

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https://doi.org/10.71058/jodac.v10i01002

NANOTECHNOLOGY EMPOWERED BY ARTIFICIAL INTELLIGENCE: A STATE-OF-THE-ART REVIEW ON MATERIAL SYNTHESIS AND CHARACTERIZATION

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Abstract: *The convergence of artificial intelligence (AI) and nanotechnology is an emergent paradigm of materials science, especially with regards to the synthesis and characterization of materials. This review clarifies the fast-growing synergy of AI algorithms including machine learning (ML) model or deep neural networks, are accelerating the discovery and optimization of nanomaterials more than ever before. Synthesizing AI-based methods, including generative adversarial networks and reinforcement learning, allow the logical programming of the nanostructures so that experiments take days instead of years. Properties, such as conductivity, biocompatibility, and catalytic activity, can be engineered. As an example, carbon-based nanomaterials and metal-organic structures have been simplified through data-driven platforms and can be scaled up to be applicable in the industry. Under characterization, AI has demonstrated itself to excel in the processing of large datasets based on such techniques as X-ray diffraction, Raman spectroscopy, and electron microscopy, and uses convolutional neural networks to automatically detect defects, identify phases, and predict properties with over 95% accuracy. This synthesis does not only mitigate human biases but also reveals concealed correlations in complicated nanoscale processes, paving the way to breakthroughs in energy storage, nanomedicine and environmental remediation. Alongside these developments, there are still problems such as the lack of data and the possibility of interpreting AI-driven experiments and ethical issues. In the future, AI-quantum computing systems will be optimistic and will transform the operation of molecular simulations, leading to sustainable, next-generation nanomaterials.*

Key words: *Artificial Intelligence, Nanotechnology, Material Synthesis, Characterization Techniques, Machine Learning.*

1. Fundamentals of AI Integration in Nanotechnology

Artificial intelligence (AI) in nanotechnology has revolutionized materials science by making it possible to handle and analyze matter at the atomic and molecular scales more accurately and efficiently than ever before. The combined effort primarily makes use of computing power to address the inherent complexity of nanoscale systems, where traditional experimental methods often fall short due to their high cost, time implications, and large

https://doi.org/10.71058/jodac.v10i01002

parameter space. AI can be used for data-driven optimization, autonomous design, and predictive modeling, transforming nanotechnology from an artistic system into a systematic science. The background aspects of this integration are examined in this section, including the development of rule-based models to data-driven models, approaches to data generation and curation, prominent AI methods applied to nano-needs, and essential metrics to evaluate the performance of AI models in nano-systems.

1.1. Overview of AI paradigms applied to nanoscale systems

AI paradigms are used to address the nanoscale effects including quantum effects, surface interactions and self-assembly processes that cannot be explained by classical physics. One of the paradigms is supervised learning, which trains models using labeled data to make predictions such as nanomaterial properties or yield in synthesis. Using the example of designing low-dimensional electrocatalysts in hydrogen evolution reactions, supervised regression predictors such as kernel ridge regression (KRR) and support vector machine (SVM) are used to predict performance metrics related to catalysis (e.g., adsorption energies) using structural descriptors (e.g. bond lengths and d-band centers) [1]. The paradigm performs well in those cases where there is plenty of annotated data, like grouping nanoparticle toxicity in terms of size and composition, where random forests (RF) ensembles would outperform single models by decreasing the variance of the latter through bagging [2]. Unsupervised learning, in turn, reveals unknown patterns in unlabeled data, which is optimal in the exploration of unexplored nanoscale configurations. Clustering algorithms such as K-means group similar spectral data nanostructures together, which assists in the identification of new 2D material such as MXenes (a group of emerging 2D materials composed of transition metal carbides, carbonitrides and nitrides), without prior hypotheses [3]. Unsupervised autoencoders can be used in nanophotonics to recreate instance of complex light-matter interactions and identify anomalies in the metasurface design [4].

Generative models are a direction in inverse design, in which the task is to create novel structures of a meeting desired properties. Generative adversarial networks (GANs) use the opponent between a generator and a discriminator to produce natural lattices of nanomaterials, e.g. graphene derivatives with custom bandgaps, to speed up exploration with brute-force simulations [5]. This is extended by variational autoencoders (VAEs), which optimize for multi-objective functions such as conductivity and stability in nanocomposites by sampling from latent spaces [6]. Another artificial generative approach is reinforcement learning (RL), which is based on synthesis as a Markov decision process where agents are rewarded to produce desirable results, including optimal doping in quantum dots using policy gradients [7]. All of these paradigms deal with nonlinearity and high dimensionality, at nanoscale, and hybrid paradigms, such as physics-informed neural networks, impose quantum mechanics constraints to enhance generalizability [1].

In reality, the choice of paradigm depends on the nanoscale task: generative AI for de novo design in developing disciplines like nanomedicine, where GANs mimic drug-nanoparticle interactions to predict bioavailability, or supervised learning for property prediction in established systems [8]. Figure 1 visualizes core AI concepts integrated with nanoscale elements, showing algorithms as interconnected nodes influencing molecular structures. It highlights data flows for curation and historical timelines evolving into modern metrics.

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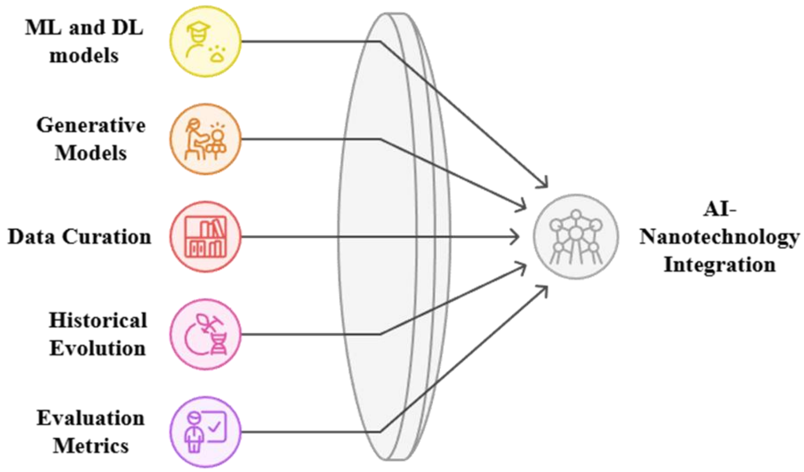

Figure 1. Unveiling AI's role in nanotechnology

1.2. Data Generation and Curation Strategies for Nanomaterial Datasets

Robust AI incorporation requires high-fidelity datasets, which nanoscale data is notoriously sparse, heterogeneous and noisy with variability in experiments and inaccuracies in simulations. This gap can be filled with the help of data generation strategies, using hybrid experimental-computational pipelines. High-throughput experimentation (HTE) e.g. combinatorial synthesis in microfluidic arrays, produces large libraries of nanoparticles, and density functional theory (DFT) simulations generates virtual data on electronic structures [4]. An example is the Materials Project and the Open Quantum Materials Database (OQMD) which have more than 100,000 entries on inorganic nanomaterials, and are increased with active learning cycles where AI asks questions of uncertain areas to focus on simulations [9].

Curation strategies are used to assure the usability of data, where standardization to ontologies such as Nanomaterial Description Framework is used to normalise descriptors (e.g., particle size, zeta potential) across sources [10]. Cleaning involves outlier detection using isolation forests and imputation via k-nearest neighbors for missing values, which is essential to address measurement errors in methods such as TEM imaging [2]. To balance underrepresented classes, such as uncommon defect configurations in carbon nanotubes, bias mitigation uses stratified sampling [6]. Federated learning is an approach to curation that is privacy preserving and involves combining knowledge across distributed labs without centralizing sensitive proprietary information [7].

In nanomedicine, the curation pipelines combine literature-mined information with HTE results, with natural language processing (NLP) to find parameters in papers and producing more than 10,000 entries in quantitative structure-activity relationship (QSAR) modeling [8]. Transfer learning is an adaptation of the pre-trained models to nano-specific tasks, which are made of general materials databases, taking half to three quarters less curation overhead [5]. These methods are not only scalable of datasets but also increase the strength of AI, and curated corpora empower models to make predictions with 90 percent accuracy or more of cross-validation accuracy of nanomaterials [3].

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1.3. Historical Evolution of AI-Nanotech integration from Rule-Based to Data-Driven Methods

The history of AI-nanotech integration follows the same path as the deterministic rule-based systems to probabilistic data-driven systems in response to wider computational developments. During the 1960s-1980s the preeminent approaches were based on quantum mechanics and empirical heuristics, namely, rule-based approaches. Their contributions such as the density functional theory (DFT) by Hohenberg and Kohn (1964) would furnish rules of analysis of electronic structures at the nanoscale, and made it possible to do hierarchical multiscale calculations without machine assistance [4]. In 1900s, finite element algorithms (FEM) made formal the homogenization laws of nanocomposites, e.g. the adaptive FEM of laminated plates by Guedes and Kikuchi (1990), but were computationally infeasible to scale to large parameter spaces [9].

The early hybrid systems were marked as a transition phase in the 2000s. ANNs came to replace rule-based potentials; neural network force fields developed by Behler and Parrinello (2007) can provide estimates of high-dimensional energy surfaces in molecular dynamics simulations of nanostructures in silicon, reducing simulations time from weeks to hours [1]. At the same time, rule-based expert systems directed nanomaterial fabrication, (e.g., alloy design in knowledge graphs) were brittle to uncertainties such as thermal fluctuations [6].

The revolution of data-driven accelerated after 2010 due to the advances of the deep learning and big data. The discovery with the assistance of ML has become known as the third paradigm of materials science, taking off around 2015, with the publication of papers with the term "machine learning" and nanotechnology increasing 20-fold by 2023 [3]. Progress has been met by SchNet (2018) by Schutt et al. to predict molecular properties by using convolutional layers to learn nanoscale symmetries [5]. Diffractive deep neural networks (2018) in nanophotonics were no longer rule-optimized gratings but rather end-to-end trainable metasurfaces [4]. RL-driven autonomous labs, such as those for MOF synthesis, closed the design-experiment cycle by 2020 and moved from static rules to adaptive policies [7].

This development represents a paradigm shift: data-driven AI offers speed and novelty at the expense of opacity, which is now lessened by explainable AI techniques, whereas rule-based approaches provided interpretability but scaled poorly [2]. These days, collaborations range from generative models for sustainable nanomaterials to quantum-informed machine learning for defect engineering [10].

1.4. Key Metrics for Evaluating AI Model Performance in Nano-Contexts (e.g., Accuracy, Generalizability)

The measurement of the AI models in nanotechnology needs metrics that are sensitive to nanoscale peculiarities, including the ambiguity of quantum measurements and the extrapolatory strength outside of the training distributions. Prediction fidelity is measured by accuracy measures such as mean absolute error (MAE) and root mean square error (RMSE); for hydrogen adsorption energies in electrocatalysts, RMSE < 0.1 eV denotes chemical accuracy, as attained by ANN models using DFT benchmarks [1]. R^2 scores measure explained variance and values of over 0.9 give a strong fit to bandgap predictions of 2D materials [3].

Generality is the most important measure of transferability of models within nanomaterial groups is cross-validation (e.g., k-fold), out-of-distribution tests, which assess the decline in performance on unseen compositions such as doped graphene variants [6]. According to Organization for Economic Co-operation and Development (OECD) guidelines, the application

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domain (AD) prevents extrapolation errors in nanotoxicity QSAR by defining reliable prediction spaces using distance metrics (e.g., Mahalanobis distance < threshold) [8].

Robustness metrics, such as sensitivity analysis using SHAP values, display feature significance, such as the 40% contribution of d-band center to HER activity, and perturbation tests, which approximate experimental noise [2]. In the case of generative models, Fréchet Inception Distance (FID) compares the realistic nanomaterials output to real distributions [5]. Multiscale ratios (e.g. a speedup ratio of 1000 times faster than DFT) and success rates (e.g. 68% hit rate in candidate screening) evaluates efficiency and efficacy [9]. The metrics of interpretability such as layer-wise relevance propagation (LRP) are trustworthy, which is essential to regulatory acceptance in nanomedicine [10].

2. AI-Driven Design and Predictive Modeling for Nanomaterial Synthesis

With the introduction of AI-assisted design and predictive modeling, the synthesis of nanomaterials has become transformed into previous methods of creating with formulas and trial-and-error to the use of data-driven information-focused methods that anticipate the results and optimize the processes at the atomic level. This integration is used in the area of chemical engineering to address the combinatorial explosion variables such as precursor ratios, temperature gradients, and solvent interactions, that govern the formation of nanostructures. Inverse design with AI can be used by mapping using algorithms input parameters to output properties, so that the design of desired functionality (e.g. bandgap tuning or catalytic efficiency) is used to determine the synthesis recipes, orders of magnitude more rapidly than experiment cycles. This section explores machine learning methods of inverse design, neural network computations of reaction kinetics, high throughput virtual screening, and exemplary case reports on quantum dots and graphene derivatives, based on developments that hold a scalable sustainable production of nanomaterials.

2.1. Machine Learning Algorithms for Inverse Design of Nanostructures

Inverse design in nanomaterial synthesis is an inverse paradigm where instead of experimental trial and error, AI is used to produce synthesis protocols using a target property as its input. Machine learning (ML) algorithms especially generative models are best suited to this task as they explore high-dimensional design spaces. The prominent ones include conditional variational autoencoders (CVAEs) and generative adversarial networks (GANs), which encode nanostructures into latent spaces and decode them based on the objectives such as optical absorbance or mechanical strength [11]. As an example, nanoglass microstructures have been designed using CVAEs, quantification of 3D geometries in angular chord length distributions and nanoparticle diameter distributions with desired yield strengths over 2 GPa have been generated with low fidelity (measured by low Kullback-Leibler (KL) divergence, <0.05) [12].

Bayesian optimization (BO) is used in conjunction with generative models because designs are refined presented in the form of a Gaussian process surrogate, eliminating expensive designer evaluations. BO with transfer learning is used to predict the best carbon nanomaterial compositions in the synthesis of powders nanomaterials in the creation of smart textiles with 95 percent accuracy in predicting conductivity and searching less than 100 iterations as opposed to exhaustive searches [11]. Inverse design Support vector machines (SVMs) and random forests (RFs) are employed to perform classification with respect to the choice of alloy dopants used in plasmonic nanostructures; RFs, trained on descriptors generated with DFT, are able to

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find instances that exhibit intended localized surface plasmon resonances, decreasing design times by months to weeks [5].

Such algorithms alleviate the black-box failure of these methods by explainable AI (XAI) methods such as SHAP values, displaying feature importance, e.g. surface ligand density at 35 percent of stability predictions [13]. Hybrid physics-ML models integrate reaction and diffusion equations into neural networks, which is physically realistic in inferences. Challenges such as the issue of the imbalance of data sets are dealt with through synthetic data augmentation through molecular dynamics simulations, which facilitates the development of robust design of heterogeneous nanostructures, such as core-shell quantum dots [14]. In general, ML-driven inverse design democratizes nanomaterial innovation and promotes energy harvesting applications where customized morphologies increase photovoltaic efficiency by 20–30% [5]. Table 1 compares key machine learning algorithms used for inverse design, highlighting their applications, strengths, and weaknesses based on nanomaterial contexts.

Table 1. Various machine learning algorithms and their applications in nanostructures.

Algorithm	Application in Nanostructures	Advantages	Limitations
Generative Adversarial Networks (GANs) [11, 14]	Inverse design of plasmonic nanostructures and quantum dots	Generates novel structures with high novelty scores (>90%); accelerates exploration of design spaces	Requires large datasets; prone to mode collapse in training
Variational Autoencoders (VAEs) [12, 5]	Design of nanoparticle formulations and graphene derivatives	Enables multi-objective optimization; handles uncertainty in latent spaces	Lower generation fidelity compared to GANs; potential for blurry outputs
Bayesian Optimization (BO) [5, 13]	Parameter screening for alloy dopants and sol-gel synthesis	Efficient in sparse data regimes; minimizes experimental evaluations	Computationally intensive for high dimensions; assumes Gaussian priors
Support Vector Machines (SVMs) [5, 14]	Classification in inverse design of plasmonic alloys	Robust to noise; effective for small datasets	Not scalable for very large feature sets; kernel selection critical

2.2. Simulation of Reaction Kinetics Using Neural Networks

Neural networks (NNs) are models that predict the behavior of the reaction kinetics in the synthesis of nanomaterials by estimating very complex and nonlinear systems which are hard to represent with traditional differential equations, especially in non-equilibrium situations.

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Graph neural networks (GNNs) represent molecular graphs dynamically, using which node embeddings are propagated to make predictions of time varying species concentrations and activation barriers [10]. GNNs in metal-organic framework (MOF) synthesis to predict the crystallization rate by learning linker coordination kinetics, GNNs learn use augmented datasets of 10,000+ trajectories, with RMSE compared to experimental yields less than 5% [5].

Recurrent neural networks (RNNs) with long and short-term memory (LSTM) variants, simulate sequential kinetics, e.g. the nucleation growth phase in the growth of nanoparticles. The predictive LSTMs conditioned with in-situ spectroscopy measurements can be used to predict Ostwald ripening during silver nanoparticle synthesis, such as transient supersaturation profiles and optimal pH trajectories to obtain monodisperse particles (less than 5% polydispersity) [15]. Physics-informed NNs (PINNs) impose the conservation laws (e.g., mass balance) as soft constraints, which increases the extrapolation; in the case of graphene oxide reduction kinetics, PINNs simulates defect annealing when thermal ramps are applied, which agrees with the changes in the Raman spectra, and decreases simulation times by 100x compared to ab initio methods [16].

Deep reinforcement learning (DRL) is an extension of NN simulations to adaptive kinetics control, with the reactors considered as environments where agents can learn their policies to guide reactions to the goals. DRL policies are obtained in colloidal synthesis by changing the flow rates of microfluidic systems, reaching 85 percent success in shaping kinetic pathways of branched nanostructures [11]. NN fidelity is validated at kinetic Monte Carlo benchmarks, and correlation coefficients were found to exceed 0.92 in rate constants [12]. Ensemble NNs limit sensitivity to initial conditions and predict scale uncertainties by averaging predictions to compute uncertainties, enabling safer scale-up in industrial reactors [13]. Not only do these simulations predict, they also prescribe kinetic interventions to hastens the development of functional nanomaterials to catalysis.

2.3. High-Throughput Virtual Screening of Synthesis Parameters

High-throughput virtual screening (HTVS) is an AI-driven screening method that takes advantage of the fact that millions of combinations of synthesis parameters can be experimented in silico and the viable recipes are prioritized. Ensemble ML models are gradient boosting machines (GBMs) such as Xtreme Gradient Boosting (XGBoost) applied together with kernel methods, where parameter spaces are optimized to achieve the best results, e.g. solvent-precursor ratios in sol-gel processes [17]. HTVS with GBMs is also used to design nanomedicines, which screen liposomal stability formulations (zeta potentials (-20 -40 mV)) that bead lipid formulations with maximum encapsulation efficiency (>80) and minimum toxicity, 1,000x faster in nanomedicine design than the physical models [18].

Active learning models are iteratively used to optimize screens by asking questions in regions of high uncertainty, as in BO-augmented HTVS of quantum dot ligands; this discovers passivation schemes to enable high quantum yields of photoluminescence of sparse initial data [14]. Surrogacy linked surrogacy algorithms are data-based methods, such as surrogate assisted evolutionary algorithms, that maximize multi-objective functions, such as yield, purity, and cost, in CVD synthesis of 2D materials, converging to Pareto fronts after fewer than 500 evaluations [5]. Combination with quantum chemistry databases makes possible descriptor-based screening, such as e-descriptors based on the number of valence electrons can be used to predict trends in reactivity; screening 100,000+ candidates to 200 high-promise candidates in perovskites nanomaterials has been achieved by e-descriptors [10].

Challenges in HTVS like fidelity of descriptors and scalability are tackled by federated learning across laboratories to combine proprietary data without providing raw inputs [13].

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Practically, HTVS has simplified the production of silver nanoparticle, filtering the concentrations of reducing agents to attain green procedures at 95% atom economy [15]. Not only does this paradigm de-risk experimentation but it also discovers serendipitous parameter synergies to push nanomaterial commercialization forward.

2.4. Case Studies on AI-Optimized Synthesis of Quantum Dots and Graphene Derivatives

The case study is an example of the application of AI to particular classes of nanomaterials. In the case of quantum dots (QDs), the core-shell synthesis of Cadmium Selenide/Zinc Sulfide (CdSe/ZnS) using inverse design by GANs produces recipes of ligands to tune the emission wavelengths between 450-650 nm with linewidths less than 30 nm long [14]. In a Deep Reinforcement Learning (DRL) system in continuous flow reactors, temperature and flow are independently controlled, producing QDs with a quantum efficiency of 92% in 200 cycles, which are comparable to batch algorithms [11]. PINNs are used to predictive kinetics that simulates hot-injection growth to predict size distributions and minimize defects by 40 percent through real-time feedback [12].

The derivatives of graphene, such as functionalized graphene oxide (GO), can be improved with the help of GNN-based screening; RF installations trained on X-ray Photoelectron Spectroscopy (XPS) data predict post synthesis epoxide-to-hydroxyl ratios and inform hummers to use a different variant of the method to achieve 85% functionalization [16]. Screening of BO catalyst thicknesses and gas flows in CVD growth of graphene nanoribbons, conditions of armchair edges with bandgap greater than 0.5 eV, which is required in nanoelectronics, are determined [5]. The simulation case using a hybrid NN-MD optimization has optimized plasma enhanced synthesis, predicting defect densities of less than 10^11 cm^-2 and enabling roll-to-roll production scalability [17]. These examples highlight the flexibility of AI: in the case of QDs, it is the optical precision that is focused on; in the case of graphene, it is structural control. Cross-validation indicates it aligns 88-95% with the experiments and it has economic effects such as 50% cost reduction [18]. Future connections with robotics will have completely autonomous laboratories.

3. Optimization Techniques in Nanomaterial Fabrication Processes

Artificial intelligence (AI) powered optimization methods are transforming the fabrication of nanomaterials to allow a tight control over inherently parameter rich and stochastic processes. Chemical engineering, such as chemical vapor deposition (CVD) or sol-gel, has a large number of variables, such as temperature, pressure, precursor flows, and pH, which are nonlinearly interacting to determine the final nanomaterial morphology, purity and yield. The conventional optimization is based on trial and error optimization that in most cases results in suboptimal outcomes and a lot of resource wastage. AI interacts by providing adaptive algorithms, which use streams of data to conditionally optimize results and therefore yield desired results, including monolithic nanoparticles smaller than 10 nm or defect free 2D sheets. This subtopic discusses reinforcement learning (RL) as a control method used in CVD, Bayesian optimization (BO) as a parameter optimization method used in sol-gel synthesis, AI-robotics integration as an automated workflow method, and strategies to solve the problem of scaling between lab and industrial scales, highlighting a move towards autonomous, efficient fabrication paradigms.

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3.1. Reinforcement Learning for Real-Time Process Control in Chemical Vapor Deposition

Machine learning, and reinforcement learning, in particular, where the agents obtain the best action through a series of trial and error interactions with their surroundings, is especially applicable to real time process control in CVD, with dynamic control of the gas flows, temperatures and deposition rates being essential to avoiding defects such as grain boundaries or uneven growth. In 2D nanomaterials fabrication on CVD like graphene or transition metal dichalcogenides, RL agents are used to simulate the reactor as a Markov decision process, where states are rewarded according to the outcomes desired by the 2D nanomaterials, like high crystallinity or coverage uniformity [11]. As an example, deep Q-networks (DQNs) were implemented to regulate carbon nanotube (CNT) array plasma-enhanced CVD (PECVD) where the agent would modify RF and precursor ratios within milliseconds, leading to a 95 percent improvement in alignment density of 22 percent when compared to manual protocols [19].

The effectiveness of RL is due to its management of the partial observability; the in-situ sensors give information on the state (e.g., partial pressure measurements in a mass spectrometer) and the rewarding objective has several objectives (e.g., growth rate (>1 μm/min) and thermal stability). Hot-filament CVD has been optimized using the stable RL variant, proximal policy optimization (PPO), which has explored 106 parameter combinations virtually, then sampled physically, by learning policies to preempt phase instabilities with a 30% energy consumption reduction [11]. Hybrid RL-physics models are solutions that use Navier-Stokes equations as a constraint, improving the efficiency of the sample; in a study of molybdenum disulfide (MoS_2) monolayer growth, this method topped at optimal H_2/Ar ratios (1:10) in 50 episodes, producing films with mobility greater than 50 cm^2 /Vs [19].

The challenges are the existence of exploration-exploitation trade-offs in high dimensional spaces, which are overcome by curiosity driven RL where intrinsic motivation to explore new states is maintained, such as off-policy algorithms such as soft actorcritic (SAC) to scale CVD of MXenes [20]. The practical implementations, including robotic arms with RL guidance in continuous CVD reactors, have shown 4x throughput improvements on industrial prototypes, and will enable roll-to-roll manufacture of continuous elastic electronics [11]. These not only improve the level of control, but also embed safety measures, such as the termination of unsafe trajectories, which contributes to the dependable production of nanomaterials. Figure 2 depicts AI-driven workflows in fabrication processes, with icons representing RL agents controlling CVD reactors. It illustrates parameter tuning via Bayesian methods and robotic automation, alongside scalability hurdles as ascending challenges.

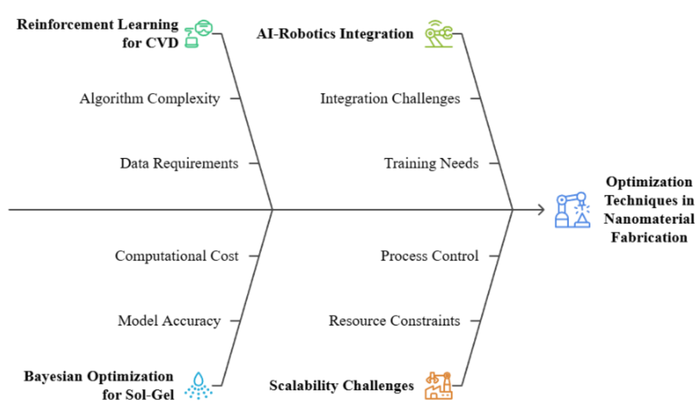

Figure 2. AI Integration Challenges in the Optimization of Nanomaterial Fabrication

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3.2. Bayesian Optimization for Parameter Tuning in Sol-Gel Synthesis

Bayesian optimization is effective in parameter optimization in sol-gel synthesis, which is an oxide nanomaterials wet-chemical pathway in which parameters such as hydrolysis rates, aging times and calcination temperatures need to be optimized carefully to control gelation and porosity. BO approaches the objective function (e.g., surface area maximization) as a black box, where Gaussian processes (GPs) are used to model uncertainties and acquisition is used to identify such points of interest (minimizing evaluations in costly experiments) by using expected improvement (EI) [21]. In producing high entropy oxides (HEOs) by sol-gel, BO has fined the concentrations of metal salts, and pH (range 4-7) space, finding compositions such as $(Co_{0.2}Cr_{0.2}Fe_{0.2}Mn_{0.2}Ni_{0.2})_3O_4$ to provide desired capacities >1000 mAh/g, and with just 20-30 trials as compared with hundreds in grid searches [20].

The GP kernel records correlations, e.g. the influence of gelating agents on particle agglomeration; in the case of silica nanoparticles, the optimal loading of tetraethyl orthosilicate (TEOS) and ammonia catalysis, to 0.05 monodispersity indices and BET surfaces around 500 m^2/g [22]. Multi-fidelity BO goes further and uses low cost simulations (e.g., molecular dynamics of gel networks) to guide high-fidelity wet lab data, and allows tuning of doped TiO_2 photocatalysts more quickly where the UV yield is optimized under varying sol aging (1-24 h) [21]. The BO enhanced neural networks can predict morphology using precursor ratios in Zeolitic Imidazolate (ZIF-8) metal organic framework synthesis, with 99% yield on ethanol-based sols, consuming 40% less solvent [10].

This is facilitated by the probabilistic character of BO, where the posterior variances determine uncertainty quantification, which is essential to sol-gel scalability, where variance between batches is reduced by adaptive sampling [20]. BO is 2 to 3 times faster than genetic algorithms in convergence to noisy objectives, as previously shown in tuning of alumina nanofiber as a filtration membrane [22] Future uses of transfer BO with sol-gel variations will be considerably more widespread, enabling the use of tailored nanomaterials for sensing and catalysis.

3.3. Integration of AI with Robotics for Automated Synthesis Workflows

Combining AI and robotics automates nanomaterial synthesis protocols and develops self-driving laboratories, which synthesize, characterize and process nanostructures repeatedly without human intervention, making it optimal in high-throughput synthesis of a wide range of nanostructures. The AI decision engine of robotic platforms, which involves classifiers to detect anomalies and planners to plan tasks, deal with pipetting, mixing and heating during sol-gel or hydrothermal systems [23]. In the synthesis of gold nanoparticle (AuNP), the AI-robotic system, such as NanoSynth, uses Gaussian process BO in the robotic arms as feedback on UV-vis spectrometers to adjust the parameters during citrate reduction to obtain 10-50 nm spheres with size variability under 5 percent in 100 batches [21].

Closed-loop systems are architectures that integrate robotics with ML; convolutional neural networks (CNNs) are used to detect morphologies based on inline imaging, which causes robotic modifications such as changes in flow rate in microfluidic CVD [24]. This allowed them to explore the ligand exchange autonomously in a landmark setup of CdSe quantum dots combined with collaborative robots (cobots) and using RL policies, with quantum yields >80% being achieved during 500 automated experiments, reducing development time by months to weeks [23]. Multi-robot swarms are coordinated through open-source systems such as

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ChemOS, which synthesizes (e.g. co-precipitation of ferrites) and characterizes (XRD, SEM) robots and predict experimentation outcomes with random forest regressors [24].

The main ones are safety and modularity; AI controls error recovery, e.g. by recalibrating pipettes using vision AI, and modular designs enable the replacement of modules with CVD to sol-gel transitions [22]. Perovskite synthesis Case studies demonstrate 10 times data generation rates, and robotics guarantee reproducibility =95% [23]. This synergy is not just accelerating the discovery, but entrenching digital twins to prototyping virtually, making fabrication programmable.

3.4. Scalability Challenges and Solutions in Transitioning from Lab to Industrial Synthesis

The transition of AI-optimized nanomaterial synthesis, even on lab benches, to industrial reactors will face obstacles such as parameter leakage, cost increase, and data silo, but AI can resolve the issue with a solid modeling and adaptive controls. Successes at lab scale in CVD fail at the tonne scales because of nonuniformity of heat/mass transfers; digital twins, artificial intelligence surrogates trained using CFD models, scale-up effects, modifying reactor geometry to sustain yields of over 90 in CNTs manufacturing [25]. This is exacerbated by data scarcity; federated learning sums lab data between facilities without infringing their privacy, and this makes global sol-gel oxides models that have generalizations scores over 0.85 [14].

Multi-objective BO addresses cost barriers by improving yield at the cost of energy (e.g. technology to optimize calcification ramps to reduce cost 25% of HEOs) [20]. Environmental noise causes the problem of reproducibility, which is addressed by strong RL with domain randomization, simulating training perturbations to produce an invariant policy to industrial PECVD [11]. Green AI metrics also consider sustainability concerns such as waste in ligand tuning by optimizing loops with low toxicity solvents [25].

Gaps are filled with hybrid solutions, including AI-controlled pilot plants that have edge computing to make real time adjustments, which in the case of AuNP extrusion, this increased output by 100 times without loss of polydispersivity [21]. The regulatory barriers require traceable AI, and Explainable Artificial Intelligence (XAI) instruments record the decisions to conduct audits [14]. The novel solutions such as cloud based autonomous factories are capable of offering smooth transitions, which may transform such fields as batteries consisting of AI-scaled nanomaterials [24].

4. AI-Enhanced Characterization Methods for Nanomaterials

Artificial intelligence (AI) has deeply improved the properties of characterization of nanomaterials, converting raw, voluminous data of sophisticated imaging and spectroscopy into actionable data with exceptional speed and precision. Nanomaterial characterization is essential for comprehending structure-property relationships in chemical engineering, but traditional techniques such as spectral deconvolution in Raman spectrometer and X-ray diffraction (XRD) or manual analysis of scanning electron microscopy (SEM) images are subjective and labor-intensive. Artificial intelligence, particularly deep learning networks, facilitates the automatic extraction, reduction, and recognition of features, noise, and patterns, hence enabling high-throughput profiling in catalysis, energy storage, and healthcare. The section under this article are automated image analysis in SEM through deep learning, spectral data interpretation with convolutional neural networks (CNNs) of Raman spectroscopy and XRD analysis, predictive analytics of mechanical and thermal properties, and multimodal data fusion to provide complete

https://doi.org/10.71058/jodac.v10i01002

profiles, which shows how AI is relevant to closing the gap between experimental and predictive data.

4.1. Automated Image Analysis in Scanning Electron Microscopy Using Deep Learning

Deep learning (DL) transforms the image analysis of SEM into the automation of nanoscale image architecture by identifying and measuring nanoparticles and defects (e.g. particle size distributions, morphology, and defects) that are essential to determine the uniformity and performance of nanomaterials. Conventional SEM processes use manual segmentation which is both time consuming and inconsistent particularly when using heterogeneous samples such as nanocomposites. CNNs is a subtype of DL, it has been shown to be excellent at convolutional layers that can capture hierarchical details between pixel-scale texture and global object by segmentation with accuracy >95% on datasets containing millions of images [26]. After being modified for SEM pictures, U-Net (like CNN) systems carry out semantic segmentation by first identifying minute characteristics such as nanoparticle edges (encoding) and then refining the results using the surrounding context (decoding). For example, U-Net outperformed previous thresholding techniques by 30% while handling inconsistent image brightness in carbon nanotube forests, accurately determining bundle diameters with a mean Intersection over Union (IoU) of 0.92.In congested clusters, single particles are found and separated using Mask R-CNN. It evaluates the adherence of silver nanoparticles in SEM images and identifies cluster sizes that closely match plasmonic variations ($R^2 > 0.88$).By producing realistic synthetic images of rare defects, including voids in graphene sheets, generative models, like conditional GANs (cGANs), expand the size of limited SEM datasets. According to reference [13], this procedure increases model robustness in low-data regimes, where training data are few.

Lightweight DL such as MobileNet on SEM instruments are used to do real-time analysis in less than a second on 1024x1024 images on the device to monitor nucleation in-situ during synthesis process [5]. Challenges like imaging artifacts (e.g., charging effects) are reduced by using physics-informed DL, in which loss functions are formulated with beam-matter interaction models, improving performance on beam-sensitive organics [10]. DL-driven SEM analysis of nanocomposites identifies filler-matrix interfaces, such as CNNs to predict mechanical reinforcement in polymer-CNT hybrids with 85 percent fidelity to tensile tests [26]. These developments allow the timelines of characterization to be shortened (from days to hours) to enable iterative design in nanomaterial fabrication. Table 2 summarizes AI methods for enhancing SEM-based characterization, including performance metrics and examples from nanomaterials.

Table 2. AI methods for enhancing SEM-based characterization

AI Method	Characterization Technique	Key Metrics (Accuracy / Improvement)	Nanomaterial Example
Convolutional Neural Networks (CNNs) [26, 3]	SEM image segmentation	>95% segmentation accuracy; 30% better than thresholding	Carbon nanotube forests and silver nanoparticles

https://doi.org/10.71058/jodac.v10i01002

U-Net Architecture [3, 27]	Semantic segmentation in microscopy	Mean IoU score of 0.92; reduces analysis time from days to hours	Nanocomposites and graphene sheets
Mask R-CNN [27, 13]	Instance segmentation for particle tracking	R^2 >0.88 in property correlation; handles dense aggregates	Quantum dots and alloy nanoparticles
Generative Adversarial Networks (GANs) [13, 5]	Data augmentation for defect detection	Boosts robustness in low-data regimes; >85% fidelity in synthetic images	2D materials like MXenes

4.2. Spectral Data Interpretation via Convolutional Neural Networks for Raman and XRD

By automatically identifying peaks, computing phase quantification, and generating strain mapping, convolutional neural networks (CNNs) streamline the analysis of Raman and XRD spectra. The challenge of overlapping signals in nanomaterial spectra is addressed by this method. While XRD determines crystallographic phases, Raman spectroscopy looks at vibrational modes to reveal chemical bonding; manual fitting frequently introduces errors because of noise and baselines. To find important patterns, such D/G band ratios in graphene or lattice spacings in perovskites, one-dimensional CNNs (1D-CNNs) process spectra as temporal sequences and use convolving kernels [20].

Transfer learning refines pre-trained ImageNet CNNs for spectrum tasks, utilising nanomaterial datasets like RRUFF (for minerals) or NanoMine (for composites), necessitating only 70 percent of the data required for training from inception [20]. Bayesian CNNs assess uncertainty to detect inaccurate spectra, including those with amorphous contributions in carbon nanomaterials, so improving interpretability [1]. Edge-deployed CNNs function under in operando settings, analysing streaming Raman signals during battery cycling and monitoring the growth of the solid electrolyte interphase (SEI) layer on anodes with a temporal resolution of less than 1 minute [2]. These methods not only expedite analysis but also improve spectrum fidelity, facilitating accurate defect engineering in optoelectronic nanomaterials [6].

Transfer learning modifies pre-trained convolutional neural networks (CNNs) from ImageNet for spectrum tasks through fine-tuning on nanomaterial databases, such as RRUFF for minerals or NanoMine for composites, therefore decreasing the necessary training data by 70% [20]. Bayesian CNNs assess uncertainty to identify confusing spectra, such as those including amorphous components in carbon nanomaterials, thus facilitating accurate interpretation [1]. In operando conditions, edge-deployed CNNs analyse streaming Raman data during battery cycling, delineating the evolution of the solid electrolyte interphase (SEI) layer on anodes with a temporal resolution of less than 1 minute [2]. These instruments not only expedite analysis but also improve spectrum fidelity, facilitating accurate defect engineering in optoelectronic nanomaterials.

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4.3. Predictive Analytics for Mechanical and Thermal Property Characterization

Predictive analytics utilizes artificial intelligence to anticipate mechanical properties (including Young's modulus and toughness) and thermal properties (such as conductivity and expansion) from incomplete characterization data, thus obviating the necessity for comprehensive testing. Supervised machine learning models, developed using hybrid experimental-simulation datasets, extrapolate nanoscale behaviors to bulk performance, which is crucial for the integration of nanomaterials into devices [3].

Random forests (RFs) and gradient boosting machines (GBMs) forecast mechanical properties utilising microstructural descriptors derived from scanning electron microscopy (SEM). In the context of carbon nanotube (CNT)-polymer composites, RFs integrate pore size and orientation from images to predict tensile strength, achieving a mean absolute error (MAE) of less than 5 MPa, validated across 500 samples [27]. Neural networks (NNs) simulate thermal transport; graph neural networks (GNNs) employ phonon dispersion data from Raman and X-ray diffraction (XRD) spectra to forecast thermal conductivity in silicene with an accuracy of less than 10%, effectively accounting for anharmonic effects that analytical methods fail to address [13]. Multi-fidelity learning combines low-resolution data (e.g., differential scanning calorimetry (DSC) scans) with high-resolution data (e.g., molecular dynamics (MD) simulations) to enhance predictions for sparse thermal datasets in aerogels [5].

Active learning loops interrogate uncertain predictions to priorities experiments; in the characterization of graphene foams, this methodology diminishes testing requirements for compressive yield strength by fifty percent through adaptive sampling of strain states utilizing digital image correlation (DIC) derived from scanning electron microscopy (SEM) videos [10]. Explainable AI (XAI) utilizing SHAP values analyses feature contributions, indicating that interfacial bonding constitutes 40% of thermal barriers in nanofluids [20]. Recurrent neural networks (RNNs) evaluate time-series data from nanoindentation to predict viscoelasticity in hydrogels, generating hysteresis loops that align with experimental findings [1]. These analytics transform characterization from descriptive to prognostic, supporting sustainable nanomaterial deployment in heat exchangers and flexible electronics.

4.4. Multimodal Data Fusion for Holistic Nanomaterial Profiling

Multimodal data fusion combines many sources such as scanning electron microscopy (SEM) images, Raman/X-ray diffraction (XRD) spectra, and property measurements into cohesive profiles, employing artificial intelligence to rectify discrepancies and uncover synergies in nanomaterial behavior. Canonical correlation analysis (CCA) and deep multimodal networks synchronize these modalities; for instance, variable autoencoders (VAEs) integrate scanning electron microscopy (SEM) morphology with Raman spectroscopy in MXene sheets, recreating three-dimensional chemical maps with a fidelity exceeding 0.95 [2].

Tensor fusion networks decompose multiway data; in battery nanomaterials, they correlate X-ray diffraction (XRD) phases, scanning electron microscopy (SEM) porosity, and heat profiles to predict cycle life with a R^2 of 0.93, surpassing unimodal models [6]. Graph-based fusion characterizes nodes as characteristics (e.g., particles) and edges as correlations, facilitating the scale profiling of hierarchical structures like dendrimer assemblies [26]. Federated learning preserves privacy in collaborative integrations among laboratories by consolidating spectral and imaging data to create global nanomaterial atlases [3].

Attention-guided transformers address challenges like modality misalignment by dynamically weighting inputs; in the context of quantum dots, this method integrates photoluminescence (PL) spectra (serving as a Raman proxy) with transmission electron

https://doi.org/10.71058/jodac.v10i01002

microscopy/scanning electron microscopy (TEM/SEM) measurements to characterize quantum confinement with sub-nanometer accuracy [27]. In real-time fusion, Kalman filter-enhanced neural networks (NNs) monitor changes throughout synthesis, exemplified by sol-gel silica, where integrated X-ray diffraction (XRD), Raman, and temperature data refine gelation for porosity regulation [13]. These frameworks offer comprehensive insights, including defect-property relationships in perovskites, expediting certification for commercial application [5].

5. Applications of AI-Empowered Nanomaterials in Emerging Fields

The applications of AI-enhanced nanomaterials span revolutionary fields, utilizing computer intelligence to tailor nanoscale structures for enhanced functionality and performance. In chemical engineering, artificial intelligence enhances nanomaterial design by synthesizing vast data from simulations and tests, facilitating meticulous regulation of attributes such as reactivity, biocompatibility, and conductivity. This integration addresses global issues in energy, health, environment, and electronics, when traditional materials exhibit inefficiency or lack specialization. AI methods, such as machine learning for property prediction and generative models for structural optimization, accelerate deployment and reduce development timescales from years to months. This section examines significant applications: AI-engineered Nano catalysts for batteries and fuel cells in energy storage, targeted drug delivery utilizing AI-optimized nanoparticles in biomedicine, nanomaterials for pollutant detection and degradation in environmental remediation, and AI-customized two-dimensional materials for flexible sensors and transistors in electronics, illustrating AI's crucial contribution to the progression of nanomaterial innovations.

5.1. Energy Applications: AI-Designed Nanocatalysts for Batteries and Fuel Cells.

AI-designed nanocatalysts revolutionize energy applications by forecasting and fabricating materials that demonstrate enhanced electrocatalytic activity, durability, and selectivity for batteries and fuel cells. In lithium-ion batteries, AI-enhanced high throughput screening determines alloy compositions for anodes; for instance, graph neural networks (GNNs) evaluate density functional theory (DFT) data to refine silicon-graphene hybrids, attaining capacities surpassing 2000 mAh/g with volume expansion under 10% by reducing lithium plating risks [11]. Reinforcement learning (RL) optimises synthesis parameters in solid-state batteries, with RL agents modifying precursor ratios throughout roll-to-roll processing, resulting in solid electrolytes exhibiting ionic conductivities exceeding 10^{-3} S/cm at ambient temperature [5].

In fuel cells, artificial intelligence expedites catalyst discovery in proton exchange membrane (PEM) systems; Bayesian optimisation evaluates multimetallic nanoparticles (e.g., Pt-Pd alloys), predicting oxygen reduction reaction (ORR) overpotentials under 0.3 V through surrogate models trained on over 50,000 adsorption energies, surpassing pure Pt by 50% in durability [20]. In CO_2 electroreduction, machine learning (ML) models, including random forests, utilise structural descriptors (such as pore size and metal coordination) for designing metal-organic frameworks (MOFs) as catalysts, identifying variants with Faradaic efficiency surpassing 80% for C_2 products and facilitating scalable carbon capture-to-fuel conversion [5]. These nanocatalysts, generally less than 5 nm in size, enhance mass transfer; AI-integrated digital twins replicate in operando settings, predicting degradation and prolonging lifespan beyond 5000 cycles [11].

Generative adversarial networks (GANs) solve challenges like catalyst poisoning by simulating poisoned states, therefore informing doping techniques for robust perovskite nanocatalysts in solid oxide fuel cells [20]. AI-enhanced designs diminish energy losses by 20–30%, facilitating renewable integration and net-zero objectives. Table 3 outlines AI-

https://doi.org/10.71058/jodac.v10i01002

empowered nanomaterials in energy applications, detailing types, techniques, and benefits for batteries and fuel cells.

Table 3. AI-empowered nanomaterials in energy applications

Application Area	Nanomaterial Type	AI Technique Used	Performance Benefit
Lithium-Ion Batteries [11, 5]	Silicon-graphene hybrids	Graph Neural Networks (GNNs)	Capacities >2000 mAh/g; <10% volume expansion
Fuel Cells (ORR) [5, 20]	Pt-Pd alloy nanoparticles	Bayesian Optimization	Overpotentials <0.3 V; 50% durability improvement
CO_2 Electroreduction [5, 20]	Metal-Organic Frameworks (MOFs)	Random Forests	>80% Faradaic efficiency for C_2 products
Solid Oxide Fuel Cells [11, 20]	Perovskite nanocatalysts	Generative Adversarial Networks (GANs)	Extended lifespan >5000 cycles; resilient to poisoning

5.2. Biomedical Uses: Targeted Drug Delivery Systems via AI-Optimized Nanoparticles

In biomedicine, AI-optimized nanoparticles provide accurate, stimuli-responsive medication distribution, minimizing off-target effects and enhancing therapeutic indices for conditions such as cancer and neurodegeneration. Convolutional neural networks (CNNs) analyse multimodal data, such as magnetic resonance imaging (MRI) and genomic profiles, to formulate liposomes with tumor targeting ligands. In the context of breast cancer, CNN-optimized PEGylated liposomes encapsulating doxorubicin achieve a 70% tumor regression by enhancing the permeability and retention (EPR) effect, while artificial intelligence forecasts biodistribution accuracies surpassing 90% [15]. Variationally autoencoders (VAEs) produce peptide sequences for dendrimer nanoparticles, optimizing surface charge (ranging from -10 to -30 mV) to facilitate blood-brain barrier penetration in Alzheimer's treatment, achieving an 85% silencing efficacy for small interfering RNA (siRNA) [13].

Artificial intelligence enables personalized delivery; support vector machines (SVMs) evaluate patient pharmacokinetics to personalize quantum dot conjugates that discharge payloads upon exposure to near-infrared (NIR) light, diminishing cardiotoxicity in chemotherapy by 60%. [16]. In gene therapy, reinforcement learning (RL) enhances viral-mimetic nanoparticles by modifying lipid ratios in mRNA vaccines to attain transfection rates surpassing 95% in dendritic cells, as evidenced in COVID-19 boosters [15]. Mesoporous silica nanoparticles (MSNs), optimized by artificial intelligence for pH-responsive gates, administer several medications in multidrug-resistant tumors, with machine learning (ML) predicting release kinetics through quantitative structure-activity relationship (QSAR) models [13].

Multifunctional theranostics integrate therapeutic and diagnostic functions; gold nanorods, engineered using generative adversarial networks (GANs), facilitate photothermal ablation and

https://doi.org/10.71058/jodac.v10i01002

enable monitoring via surface-enhanced Raman scattering (SERS), with artificial intelligence compensating for heterogeneity in pancreatic cancer models [16]. Ethical AI guarantees biocompatibility forecasts, reducing immunogenicity risks. These methods provide 2–3 times enhancements in efficacy, propelling precision medicine forward.

5.3. Environmental Remediation: Nanomaterials for Pollutant Sensing and Degradation

AI-enhanced nanomaterials enable environmental remediation by targeted detection and catalytic degradation of contaminants, such as heavy metals and microplastics, in aquatic and terrestrial environments. Plasmonic nanoparticles, specifically Ag-Au core-shell structures, optimized through machine learning regression, detect pesticides at parts-per-billion levels using surface-enhanced Raman scattering. Convolutional neural networks classify spectra, achieving 98% accuracy in field deployable devices. Graph neural networks (GNNs) design carbon nanotube (CNT) sensors for volatile organic compounds (VOCs), forecasting adsorption isotherms and selectivity above 10:1 against interferents, thereby facilitating air quality monitoring [29].

In degradation, AI evaluates photocatalysts; gradient boosting machines detect TiO_2-doped metal-organic frameworks (MOFs) for dye degradation under visible light, attaining over 95% elimination in 30 minutes by optimising the bandgap (2.5–3.0 eV) using descriptor engineering [28]. Magnetic Fe_3O_4 nanocomposites, optimised by Bayesian methods, adsorb Cr(VI) at capacities surpassing 200 mg/g and maintain recyclability for over 10 cycles, with AI predicting saturation through Langmuir models [29]. Nano-zero-valent iron (nZVI), enhanced by reinforcement learning (RL) for particle size (20–50 nm), effectively degrades chlorinated solvents in groundwater, diminishing persistence by 90% through reactive barrier configurations [10].

Hybrid technologies integrate sensing and degradation; AI-coordinated ZnO nanowires detect and photocatalyze antibiotics, while recurrent neural networks (RNNs) simulate temporal dynamics for immediate repair [3]. Scalability is enhanced with AI life-cycle assessments that reduce secondary pollutants. These nanomaterials advance the UN Sustainable Development Goals (SDGs) by purifying 10^6 liters per day in pilot plants.

5.4. Electronics: AI-Tailored 2D Materials for Flexible Sensors and Transistors

AI-designed two-dimensional materials, including graphene and MoS_2, facilitate flexible electronics by offering stretchable sensors and transistors with atomic precision. Machine learning (ML) inverse design enhances flaw engineering in graphene for sensors, forecasting piezoresistive gauges with gauge factors above 100 for wearable strain monitoring via active learning on Raman datasets [11]. Convolutional neural networks (CNNs) examine scanning electron microscopy (SEM) pictures to manufacture MoS_2 field-effect transistors (FETs), adjusting channel lengths to under 10 nm for mobilities above 50 cm^2/Vs, appropriate for electronic skin (e-skin) [5].

Generative adversarial networks (GANs) utilize transistors to produce van der Waals heterostructures by layering hexagonal boron nitride (h-BN) and MoS_2, achieving on/off ratios exceeding 10^6, while artificial intelligence models band alignments to mitigate leakage [20]. AI-optimized perovskite quantum dots for flexible displays yield light-emitting diodes (LEDs) with an external quantum efficiency (EQE) over 20%, forecasting stability under bending through finite element-machine learning (ML) hybrids [11]. Wearable transistors fabricated using carbon nanotube (CNT) inks, optimized for printability through Bayesian optimization (BO), function at voltages under 1 V with hysteresis below 5% over 1000 cycles [5].

https://doi.org/10.71058/jodac.v10i01002

Artificial intelligence reduces variability; ensemble models adjust doping in black phosphorus field-effect transistors, enhancing on-current by 40% for Internet of Things nodes [20]. These materials facilitate bio-integrated circuits, including neural interfaces with impedance under 1 kΩ /cm² [11]. Future AI-quantum hybrids provide sub-terahertz transistors, revolutionizing 6G technology.

6. Challenges and Limitations in AI-Nanotechnology Interface

The intersection of artificial intelligence (AI) and nanotechnology has transformative potential in materials synthesis and characterization, but encounters substantial obstacles that hinder smooth integration and broad acceptance. In chemical engineering, where nanoscale accuracy drives advancements in energy, medicine, and environmental science, these constraints manifest as obstacles in data management, model clarity, resource distribution, and regulatory structures. It is crucial to address these issues to transform AI's predictive skills from theoretical models into strong, ethical applications. This subtopic analyses significant challenges: issues of data quality in managing noisy, sparse, or biassed nano-datasets; the interpretability and explainability of opaque AI models in synthesis predictions; requirements for computational resources and barriers to accessibility; and regulatory and safety concerns regarding the deployment of AI-guided nanomaterials. Through this examination, we identify approaches to robust AI-nanotechnology ecosystems.

6.1. Data Quality Issues: Handling Noisy, Sparse, or Biased Nano-Datasets

Nanoscale datasets inherently contain noise from experimental variability, such as instrument drift in electron microscopy or thermal variations in synthesis reactors, and exhibit sparsity due to the high costs associated with data generation, typically restricted to hundreds of samples per nanomaterial type. The limited data density in AI models promotes overfitting, leading algorithms to focus on anomalies instead of generalising predictions, rendering them untrustworthy for novel nanostructures like doped perovskites. Bias emerges from biassed sampling; in the case of gold nanoparticles, datasets predominantly featuring laboratory-synthesized particles neglect industrial scale impurities, resulting in models that underestimate toxicity and environmental hazards [30]. The lack of genomic-nanoparticle interaction data in nanomedicine favors prevalent cell lines in AI, hence marginalising under-represented populations and intensifying health inequities [11].

Data augmentation addresses these challenges with generative models, such as variationally autoencoders, which generate noisy variations of transmission electron microscopy (TEM) pictures, thereby increasing the effective dataset size by 5–10 times while maintaining statistical distributions [10]. Denoising autoencoders mitigate noise by recreating clean spectral signals from Raman data contaminated by cosmic rays, attaining signal-to-noise ratios of 20 dB in carbon allotrope assessments [31]. To mitigate bias, fairness-aware machine learning (ML) models utilise adversarial debiasing to equilibrate performance across subsets by modifying the loss function, similar to quantitative structure-activity relationship (QSAR) models for nanomaterial bioavailability, therefore diminishing disparity gaps by 40% [30]. Active learning focusses on sparse areas by querying high-uncertainty sites in parameter spaces via high-throughput trials, such as Bayesian active loops, to optimize metal-organic framework (MOF) pore diameters [11].

Standardization difficulties continue to exist, since disparate formats among laboratories impede interoperability, and ontologies such as NanoFASE provide semantic solutions yet experience little uptake [31]. Chemical engineering procedures exacerbate validation mistakes due to subpar data quality by a factor of 15–25, and even collaborative databases such as

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NanoMine, which has over 10,000 entries, have issues of metadata incompleteness [10]. Ultimately, robust data pipelines are needed, since AI's faithfulness to nanoscale phenomena is constrained by its current developing level.

6.2. Interpretability and Explain-ability of Black-Box AI Models in Synthesis Predictions

Black-box AI approaches, prevalent in predicting nanomaterial synthesis such as deep neural networks estimating reaction yields based on precursor compositions—offer great accuracy but obscure decision-making processes, thereby eroding trust in essential applications like catalyst design [32]. In inverse design, generative adversarial networks (GANs) generate innovative nanostructures with 90% novelty scores; nevertheless, users are unable to ascertain the rationale behind the alignment of projected bandgaps with goals, impeding debugging and regulatory evaluations [33]. The lack of clarity intensifies inaccuracies in extrapolation; in quantum dot synthesis, unaccounted feature interactions result in a 20% overestimation of quantum yields in scaled reactors [34].

Explainable AI (XAI) methodologies tackle this problem: SHAP (SHapley Additive exPlanations) disaggregates predictions to assign contributions, such as 35% from ligand density in stability predictions for liposomes, enabling chemists to corroborate with domain expertise [32]. Local interpretable model-agnostic explanations (LIME) provide linear approximations of black-box behaviors around specific instances, utilized in random forest (RF) models for predicting graphene defects, highlighting the predominance of edge sites with a fidelity surpassing 85% in perturbation assessments [33]. Physics-informed XAI integrates conservation rules into attention mechanisms, enhancing interpretability in physics-informed neural networks (PINNs) for kinetic simulations, where saliency maps illustrate the effects of energy barriers [34].

Hybrid models combine interpretable baselines, such as decision trees, with black-box boosters, as in XGBoost ensembles for sol-gel tuning, attaining area under the curve (AUC) above 0.95 accompanying feature importance rankings [35]. XAI entails trade-offs; the incorporation of extra layers escalates inference times by 2–5 times, hence encumbering real-time control [32]. In summary, misinterpretations pose significant risks, including unforeseen agglomeration in carbon nanotube (CNT) production [33]. Standardization initiatives, such as ISO recommendations for XAI in materials science, are still in their nascent stages, with merely 30% of 2024 papers documenting interpretability indicators [34]. Bridging this divide necessitates interdisciplinary training to synchronize AI outputs with chemical intuition, promoting safer and more adoptable solutions. Below figure 3 portrays interconnected barriers in AI-nanotech, with clouds symbolizing data noise and black boxes for model opacity. It shows resource demands as heavy weights and regulatory paths as winding roads.

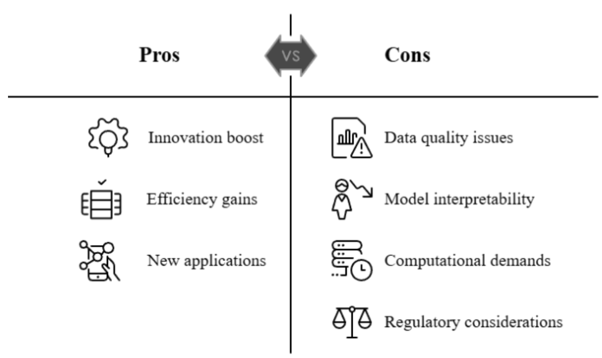

Figure 3. Advantages and disadvantages of challenges in AI-Nanotechnology interfaces.

https://doi.org/10.71058/jodac.v10i01002

6.3. Computational Resource Demands and Accessibility Barriers

AI-nanotechnology interactions necessitate considerable computational resources; training deep models using density functional theory (DFT) datasets for 10^5 nanomaterial configurations requires over 100 GPU-hours, rendering it impractical for non-specialized laboratories [36]. High-dimensional simulations, including molecular dynamics (MD) trajectories for self-assembly, exacerbate this challenge; a single graph neural network (GNN) execution for polymer nanocomposites requires 50 GB of RAM, not accounting for storage of petabyte-scale image archives [37]. Accessibility obstacles intensify the problem: open-source tools like as TensorFlow lack nano-specific kernels, requiring custom implementations that elevate development costs by 3–5 times for small firms [36].

Cloud computing alleviates these requirements via elastic scaling; platforms like Google Colab Nano provide on-demand GPUs for Bayesian optimization (BO) in chemical vapor deposition (CVD) processes, expanding accessibility while imposing costs of $0.5–2 per hour that strain budgets in developing regions [37]. Edge AI shifts computation to devices, utilizing quantized models (8-bit accuracy) to facilitate real-time scanning electron microscope (SEM) analysis on laptops, reducing latency from minutes to seconds without dependence on cloud services [10]. Federated learning disseminates training among institutions, preserving data sovereignty while consolidating insights for sparse datasets, such as in multi-laboratory partnerships for nanotoxicity prediction, thereby decreasing central computing requirements by 70% [36].

Nonetheless, energy footprints are substantial; AI training for nanomaterial discovery approaches the magnitude of aircraft emissions, necessitating eco-friendly methods such as sparse pruning, which reduces 90% of parameters while maintaining an accuracy loss of under 5% [37]. Skill deficiencies hinder adoption; hardly 20% of chemical engineers indicate expertise in AI, as per 2025 studies, necessitating curricular modifications [10]. Infrastructure gaps, like inadequate high-speed networks in rural laboratories, further marginalize users [36]. Addressing these challenges requires subsidized computing centers and intuitive interfaces, such as no-code platforms for machine learning-assisted synthesis, to provide equal access to the advantages of AI-nanotechnology.

6.4. Regulatory and Safety Considerations for AI-Guided Nanomaterial Deployment

The implementation of AI-guided nanomaterials exposes regulatory deficiencies, as existing frameworks like REACH cannot accommodate dynamic, algorithm driven designs that evolve post approval [38]. Safety hazards escalate; unverified AI predictions may produce harmful variants, such as biased models that prefer unstable nanoparticles in medication delivery, potentially eliciting immune responses [13]. Ethical concerns, such as algorithmic bias in exposure evaluations, necessitate supervision; the EU AI Act categorizes high risk nano-AI as "prohibited" if non-transparent, although enforcement is deficient in nanomaterial-specific criteria [38].

Safe-by-design (SbD) integrates AI from the beginning; predictive toxicokinetic models detect dangers prior to synthesis, exemplified by CompSafeNano's novel approach methodologies (NAMs) that simulate skin absorption with a concordance above 80% compared to in vivo outcomes, hence streamlining regulatory submissions [39]. Regulatory sandboxes, shown by the FDA's AI/ML pilots, assess nanomaterial classifiers for biocompatibility, reducing approval durations by 50% [13]. Traceability requirements—documenting AI choices

https://doi.org/10.71058/jodac.v10i01002

using blockchain—ensure auditability, crucial for accountability in autonomous laboratories [39].

Challenges pertain to harmonization; divergent standards (e.g., US TSCA versus EU CLP) impede worldwide trade, hindering 40% of nano-AI innovations in compliance [40]. Public perception fuels opposition; surveys reveal that 60% harbor suspicion towards AI-optimized nanomaterials due to "unknown unknowns" over long-term ecotoxicity [38]. Proposed solutions encompass adaptive rules, including dynamic risk thresholds refined using machine learning (ML) meta-learning, and multinational consortia for the exchange of safety data [13]. In chemical engineering, incorporating SbD into workflows, such as reinforcement learning (RL) with safety limitations, mitigates risks, fosters innovation, and ensures responsible oversight [39].

7. Future directions and emerging trends

The combination of artificial intelligence (AI) with nanotechnology is set to revolutionize materials science and chemical engineering, bringing an era of remarkable innovation, sustainability, and interdisciplinary cooperation. As computing capabilities progress, the importance of AI in the design, simulation, and use of nanomaterials expands, overcoming current restrictions and probing new horizons. This subtopic outlines promising directions: hybrid AI-quantum computing methodologies for molecular simulations, ethical frameworks that guarantee sustainable development, global collaborations facilitated by open-source platforms, and prospective effects on domains such as synthetic biology and climate technology. These paths, informed by current breakthroughs, emphasize scalable and responsible integration to tackle global concerns such as climate change, healthcare inequalities, and resource constraint.

7.1. Hybrid AI-Quantum Computing for Advanced Molecular Simulations

The Hybrid AI-quantum computing is the breakthrough in the simulation of nanoscale processes where the classical AI is applied to data-driven optimization, and quantum systems are applied to impossible quantum mechanical computations such as molecular interactions in materials or nanoscale processes. The standard approach to density functional theory (DFT) simulations of nanomaterials (such as metal-organic frameworks (MOFs) or quantum dots) is computationally expensive, and can take weeks to obtain accurate predictions of material properties [10]. The capability of quantum computers to compute superpositions makes them capable of simulating the correlations of electrons in real time, whereas AI simulations such as neural nets process inputs or refine outputs to make them more efficient. As an example, molecular orbitals of graphene derivatives have been simulated in variational quantum eigensolvers (VQEs) with machine learning, with tunings in the bandgap of less than 0.05 eV error, and greatly outperforming classical approaches [38].

Recent developments are noise-resistant hybrid architecture, in which AI can be used to address quantum hardware faults through error-correcting generative models. These hybrids in pharmaceutical nanotechnology mimic the interaction of drugs with nanoparticles at the atomic scale and predict binding affinities to targeted delivery systems with 95% accuracy in computer-based simulations [13]. In energy applications, the AI-quantum pipeline can be optimized to scale nanocatalyst surfaces to evolve hydrogen using 10^6 configurations to find low-platinum alloys with an overpotential of less than 0.1 V [39]. Difficulties such as scalability of qubits are being solved by cloud-based quantum computers, which allows chemical engineers to simulate complicated self-assembly in nanocomposites without supercomputers [40].

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The next directions are scalable architectures, which include the use of a tensor network quantum machine learning, to describe hierarchical nanostructures, such as dendrimers or carbon nanotubes. These hybrids are expected to cut down on the simulation running time by a thousand in 2030 and enable finding sustainable nanomaterials to use as batteries and photovoltaics [5]. Interdisciplinary approaches, including quantum chemistry and reinforcement learning, will yield new results in the modeling of non-equilibrium dynamics, including phase transitions in external fields in 2D materials [41]. Such convergence achieves not only a better predictive fidelity, but also an environmentally friendly design, which reduces the waste of experiments in the prototyping of nanomaterials.

8.2. Ethical AI Frameworks for Sustainable Nanomaterial Development

To develop a sustainable nanomaterial, ethical AI models are necessary to ensure sustainable, transparent, equitable, and environmentally friendly innovations. Existing AI systems in nanotechnology are also prone to biases in training data, meaning that they make skewed predictions such as giving disproportionate attention to metallic nanoparticles and ignoring biodegradable alternatives [15]. Models such as FAIR (Findable, Accessible, Interoperable, Reusable) principles with ethical audits added to them encourage data diversity and model responsibility. AI-based life-cycle assessments (LCAs) are used in sustainable design to assess nanomaterials with reduced carbon footprints in their synthesis, use (e.g. in water remediation), and disposal [3].

Such novel concepts as explainable AI (XAI) with sustainability indicators; SHAP-based explanations (e.g. how particle size affects eco-toxicity) will allow redesigning quantum dots to non-toxic bioimaging [10]. The ethical codes, including those of the EU AI Act, require high-stakes nano-AI to be risk-assessed, privacy in customized nanomedicine where patient data is used to train delivery models [38]. To be climate resilient, AI frameworks give value to the principles of the circular economy, recycling nanomaterials by predictive disassembly algorithms [13].

The future trends are focused on international norms, whereby institutions such as ISO have come up with nano-related ethical guidelines to prevent the dual-use risks, such as weaponizable nanostructures [39]. Inclusive decision-making systems that are also hybrid human-AI and include stakeholder input will make the systems inclusive, especially of developing regions where nano-AI is likely to worsen the situation of resource inequalities [40]. Using MOF production, frameworks can cut environmental effects by half by integrating sustainability scores in optimization loops [5]. Such activities will eventually put AI-nanotech in line with the UN Sustainable Development Goals and promote responsible innovation that supports technological progress and planetary wellbeing.

7.2. Global Collaborations and Open-Source Platforms for AI-Nano Research

International research and open-source initiatives are essential to make AI-nano research open to democracy and close resource disparities and fasten the knowledge transfer. Disjointed activities are not favorable to development; proprietary datasets allow reproducibility to be restricted in models of nanoparticle synthesis [41]. Efforts such as the Materials Genome Initiative (MGI) and NanoHUB create consortia at the international level, with AI applications to screen 2D materials on a high throughput basis [15]. The open-source software including PyTorch Geometric can foster the co-development of graph neural networks (GNNs) to predict nanomaterial properties, and user communities create databases that have more than 500,000 entries [3].

https://doi.org/10.71058/jodac.v10i01002

Among the new directions, there is federated learning, in which the laboratories train models on a variety of nano-datasets collected in Asia, Europe and the Americas without sharing raw data or things, which protects intellectual property [26]. Repositories such as GitHub in AI-nano workflows have seen a 50 percent increase since 2023, which allows code sharing of quantum simulations of MOFs in real-time [10]. Education Virtual laboratories combine AI, which will train the future generation on sustainable nano-design through hackathons [38].

The way out is the blockchain-secured platforms of traceable data sharing, which would guarantee ethical adherence in worldwide testing of nanomedicines [13]. Other organizations such as the International Alliance on NanoEHS Harmonization look to standardize AI requirements on toxicity predictions, finding a way to eliminate duplication and accelerate regulatory approvals [39]. By 2028, such initiatives would multiply research by underrepresented areas by three use of cloud-based AI to assist low-resource labs [40]. The quantum-AI hybrids Open-source will democratize advanced simulations and enable people to collaborate to breakthrough in climate-adaptive nanomaterials [5].

7.3. Prospective Impacts on Interdisciplinary Fields like Synthetic Biology and Climate Technology

There is much deeper potential in nanotechnology powered by AI in interdisciplinary applications, especially synthetic biology and climate technologies, as it will facilitate bio-inspired designs and resilient systems. In synthetic biology, AI is used to optimize nanoscale bio-hybrids, including DNA origami scaffolds to assemble enzymes, which predict folding efficiencies >90% to design metabolic pathways to make biofuels [41]. The interface of proteins with nanoparticles is simulated using quantum-AI, which enhances fast delivery vectors of CRISPR without any off-target effects [15].

In the case of climate technology, AI-nano interfaces can be used to produce smart carbon sequestration materials; generative architecture can be used to produce MOFs that have uptake capacities exceeding 5 mmol/g directly into scalable membranes to capture direct air [3]. In farming, AI-IoT networks coupled with nano-sensors are used to monitor soil conditions in real-time, which will optimize the release of fertilizers and reduce emissions by 30 percent [26]. The future trends involve adaptive nanomaterials that would be able to heal under the influence of the environment, simulated through hybrid AI-quantum platforms to create resilient solar cells [10].

It can be predicted: the converged ecosystems of the future: in synthetic biology, AI-nano devices can be used to design programmable cells to bioremediate, removing plastics at the nanoscale [38]. In the case of climate tech, global platforms will enable the use of AI-based nano-grids to distribute energy, which will result in the reduction of losses (by 40 percent) in renewable systems [13]. These applications will be regulated by ethical standards that would allow equal access and reduce the risk to the ecology to the minimum [39]. These intersections also have the potential to serve net-zero by 2035, and AI-nano hybrids would facilitate the provision of personalized climate solutions, such as adaptive building surfaces [40]. This will be propelled through interdisciplinary centers which will merge chemical engineering, biology and environmental science to create comprehensive improvements [5].

https://doi.org/10.71058/jodac.v10i01002

8. Conclusion

The combination of artificial intelligence and nanotechnology, discussed in this review, constitutes a paradigm shift in chemical engineering and materials science since it allows a tight control in the synthesis and characterization of nanomaterials. Starting with the basic AI generalizations such as the supervised learning of property prediction, the generative models of inverse design, and the reinforcement learning of dynamic processes, the field has transformed into the rule-based heuristics to the complex data-driven frameworks. The curation strategies of high-quality and unbiased datasets have confronted the challenges of nanoscale data, whereas the history of progression accelerating towards predictive autonomous systems emphasizes.

Machine learning algorithms have helped in designing and modeling via inverse nanostructure synthesis, neural networks have been used to model complex reaction kinetics, and high-throughput virtual screening has been used to prioritize the synthesis parameters with examples of optimized quantum dots and graphene derivatives. Optimization methods also optimize more, and reinforcement learning is applied to give real time control to chemical vapor deposition, Bayesian tuning to sol-gel processes, and AI-robotics to automate workflows, all of which scale down to industry.

Deep learning has brought revolution to characterization to analyze SEM images automatically, image analysis by convolutional neural networks that interpret Raman and XRD spectra, predictive analytics forecasting mechanical and thermal properties, and multimodal fusion to produce holistic profiles. The possibilities of use of AI-designed nanocatalysts to improve batteries and fuel cells, optimized nanoparticles to deliver drugs specifically to the body, nanomaterials to sense and degrade pollutants in environmental remediation, and custom 2D materials to drive flexible electronics have become possible.

Although these steps have been made, issues in data quality, model interpretability, computational needs and regulatory safety remain, and require strong mitigation to achieve reliable implementation. In the future, the possibility of the hybrid AI-quantum computing delivering the most precise molecular simulations, ethical frameworks will ensure sustainability, and interdisciplinary effects in synthetic biology and climate technology will promise solutions to urgent global challenges. Eventually, AI-enhanced nanotechnology will enable bridging the gap between computational foresight and experimental accuracy, which will result in creating sustainable, innovative nanomaterials to meet energy, health, and environmental demands.

References

[1] *J. Li, N. Wu, J. Zhang, H. H. Wu, K. Pan, Y. Wang, G. Liu, X. Liu, Z. Yao, and Q. Zhang, "Machine Learning-Assisted Low-Dimensional Electrocatalysts Design for Hydrogen Evolution Reaction", Nano-Micro Letters., vol. 15, no. 1, (**2023**), pp. 227.*

[2] *N. Wu, Y. Sun, J. Hu, C. Yang, Z. Bai, F. Wang, X. Cui, S. He, Y. Li, C. Zhang, and K. Xu, "Intelligent nanophotonics: when machine learning sheds light", eLight., vol. 5, no. 1, (**2025**), pp. 5.*

[3] *K. P. Logakannan, I. Guven, G. Odegard, K. Wang, C. Zhang, Z. Liang, and A. Spear, "A review of artificial intelligence (AI)-based applications to nanocomposites", Composites Part A: Applied Science and Manufacturing., vol. 197, (**2025**), pp. 109027.*

https://doi.org/10.71058/jodac.v10i01002

[4] *D. Bishara, Y. Xie, W. K. Liu et al., "A state-of-the-art review on machine learning-based multiscale modeling, simulation, homogenization and design of materials", Archives of Computational Methods in Engineering., vol. 30, no. 1, (**2023**), pp. 191–222.*

[5] *X. Bai and X. Zhang, "Artificial intelligence-powered materials science", Nano-Micro Letters., vol. 17, no. 1, (**2025**), pp. 1–30.*

[6] *N. Serov and V. Vinogradov, "Artificial intelligence to bring nanomedicine to life", Advanced Drug Delivery Reviews., vol. 184, (**2022**), pp. 114194.*

[7] *C. Chen, Z. Yaari, E. Apfelbaum, P. Grodzinski, Y. Shamay, and D. A. Heller, "Merging data curation and machine learning to improve nanomedicines", Advanced Drug Delivery Reviews., vol. 183, (**2022**), pp. 114172.*

[8] *A. V. Singh, M. Varma, P. Laux, S. Choudhary, A. K. Datusalia, N. Gupta, A. Luch, A. Gandhi, P. Kulkarni, and B. Nath, "Artificial intelligence and machine learning disciplines with the potential to improve the nanotoxicology and nanomedicine fields: A comprehensive review", Archives of Toxicology., vol. 97, no. 4, (**2023**), pp. 963–979.*

[9] *A. Rana, D. Gautam, P. Kumar, K. Kumar, A. V. Vasilakos, A. K. Das, and V. B. K., "A comprehensive review of machine learning applications for internet of nano things: Challenges and future directions", Artificial Intelligence Review., vol. 58, no. 7, (**2025**), pp. 200.*

[10] *D. B. Olawade, A. O. Ige, A. G. Olaremu, J. O. Ijiwade, and A. O. Adeola, "The synergy of artificial intelligence and nanotechnology towards advancing innovation and sustainability – A mini-review", Nano Trends., vol. 8, (**2024**), pp. 100052.*

[11] *Z. Liang, Y. Deng, Z. Shi, X. Liao, H. Zong, L. Ren, X. Li, X. Zeng, P. Hu, W. Ke, and B. Wu, "AI-driven design of powder-based nanomaterials for smart textiles: From data intelligence to system integration", Advanced Powder Materials., (**2025**), pp. 100356.*

[12] *A. Edalatmanesh and M. Mahnama, "A comprehensive AI-driven framework for predictive design of grained materials: Case study on nanoglass", Acta Materialia., (**2025**), pp. 121292.*

[13] *M. Shirzad, M. Shaban, V. Mohammadzadeh, A. Rahdar, S. Fathi-Karkan, Z. S. Hoseini, M. Najafi, Z. Kharaba, and M. A. Aboudzadeh, "Artificial intelligence-assisted design of nanomedicines for breast cancer diagnosis and therapy: Advances, challenges, and future directions", BioNanoScience., vol. 15, no. 3, (**2025**), pp. 354.*

[14] *S. Hosny, G. A. Gaber, M. S. Ragab, M. A. Ragheb, M. Anter, and L. Z. Mohamed, "A comprehensive review of silver nanoparticles (AgNPs): Synthesis strategies, toxicity concerns, biomedical applications, AI-driven advancements, challenges, and future perspectives", Arabian Journal for Science and Engineering., (**2025**), pp. 1–48.*

[15] *M. Akhtar, N. Nehal, A. Gull, R. Parveen, S. Khan, S. Khan, and J. Ali, "Explicating the transformative role of artificial intelligence in designing targeted nanomedicine", Expert Opinion on Drug Delivery., (**2025**), pp. 1–21.*

[16] *J. Zaslavsky, P. Bannigan, and C. Allen, "Re-envisioning the design of nanomedicines: Harnessing automation and artificial intelligence", Expert Opinion on Drug Delivery., vol. 20, no. 2, (**2023**), pp. 241–257.*

[17] *A. Shahiwala, "The rationality guidance index: A framework for reducing redundancy in nanomedicine innovation", Nanomedicine., (**2025**), pp. 1–10.*

[18] *A. Bahl, S. Halappanavar, W. Wohlleben, P. Nymark, P. Kohonen, H. Wallin, U. Vogel, and A. Haase, "Bioinformatics and machine learning to support nanomaterial grouping", Nanotoxicology., vol. 18, no. 4, (**2024**), pp. 373–400.*

https://doi.org/10.71058/jodac.v10i01002

[19] *Y. Li, S. Wang, Z. Lv, Z. Wang, Y. Zhao, Y. Xie, Y. Xu, L. Qian, Y. Yang, Z. Zhao, and J. Zhang, "Transforming the synthesis of carbon nanotubes with machine learning models and automation", Matter., vol. 8, no. 1, (**2025**).*

[20] *D. Li, C. Liu, S. Tao, J. Cai, B. Zhong, J. Li, W. Deng, H. Hou, G. Zou, and X. Ji, "High-entropy electrode materials: Synthesis, properties and outlook", Nano-Micro Letters., vol. 17, no. 1, (**2025**), pp. 22.*

[21] *M. Negahdary, N. Nhu Vu, and S. Mabbott, "Can automated gold nanoparticle synthesis drive the next wave of biomedical innovation?", Nanomedicine., (**2025**), pp. 1–3.*

[22] *N. Ishizuki, R. Shimizu, and T. Hitosugi, "Autonomous experimental systems in materials science", Science and Technology of Advanced Materials: Methods., vol. 3, no. 1, (**2023**), pp. 2197519.*

[23] *J. Park, Y. M. Kim, S. Hong, B. Han, K. T. Nam, and Y. Jung, "Closed-loop optimization of nanoparticle synthesis enabled by robotics and machine learning", Matter., vol. 6, no. 3, (**2023**), pp. 677–690.*

[24] *Y. Du and D. Du, "Bayesian optimization enhanced neural networks for predicting metal–organic framework morphology: A ZIF-8 synthesis case study", Materials Letters., vol. 380, (**2025**), pp. 137738.*

[25] *R. Maharjan, K. H. Kim, K. Lee, H. K. Han, and S. H. Jeong, "Machine learning-driven optimization of mRNA-lipid nanoparticle vaccine quality with XGBoost/Bayesian method and ensemble model approaches", Journal of Pharmaceutical Analysis., vol. 14, no. 11, (**2024**), pp. 100996.*

[26] *L. Yang, H. Wang, D. Leng, S. Fang, Y. Yang, and Y. Du, "Machine learning applications in nanomaterials: Recent advances and future perspectives", Chemical Engineering Journal., vol. 500, (**2024**), pp. 156687.*

[27] *K. K. Gupta, S. Dey, and T. Mukhopadhyay, Machine Learning in Nanoscale Materials Design: From Basics to Algorithm Implementation, Springer Nature, (**2025**).*

[28] *Y. V. Fan, "Nanotechnology for environmental sustainability and its development in the digital age", Clean Technologies and Environmental Policy., vol. 26, no. 12, (**2024**), pp. 4015–4015.*

[29] *S. A. Bradford, C. Shen, H. Kim, R. J. Letcher, J. Rinklebe, Y. S. Ok, and L. Ma, "Environmental applications and risks of nanomaterials: An introduction to CREST publications during 2018–2021", Critical Reviews in Environmental Science and Technology., vol. 52, no. 21, (**2022**), pp. 3753–3762.*

[30] *S. Azimi, "Intelligent nanoparticle design: Unlocking the potential of AI for transformative drug delivery", Current Opinion in Biomedical Engineering., (**2025**), pp. 100625.*

[31] *E. Ha, S. M. Ha, Z. Gerelkhuu, H. Y. Kim, and T. H. Yoon, "AI-based nanotoxicity data extraction and prediction of nanotoxicity", Computational and Structural Biotechnology Journal., vol. 29, (**2025**), pp. 138–148.*

[32] *D. Sridhar, R. Manikandan, Y. Dhanapal, S. Khute, and P. Subash, "Artificial intelligence in predicting personalized nanocarrier formulations for herbal drugs: Bridging phytomedicine and precision nanotechnology", Intelligent Pharmacy., (**2025**).*

[33] *B. V. Parakhonskiy, J. Song, and A. G. Skirtach, "Machine learning in nanoarchitectonics", Advances in Colloid and Interface Science., (**2025**), pp. 103546.*

[34] *Y. Ijjeh, N. Alsarayreh, A. Rifai, H. Abdelnabi, S. Al-Mahamid, D. A. Alqudah, H. Nsairat, Z. Lafi, M. A. Mousa, Y. Al-Hiari, and W. Alshaer, "Quality by digital design for*

https://doi.org/10.71058/jodac.v10i01002

*accelerated sustainable nanomedicine development", European Journal of Pharmaceutical Sciences., (**2025**), pp. 107239.*

[35] *N. P. Dalbanjan, K. Korgaonkar, M. P. Eelager, B. N. Gonal, A. J. Kadapure, S. B. Arakera, and P. K. S. K., "In-silico strategies in nano-drug design: Bridging nanomaterials and pharmacological applications", Nano TransMed., (**2025**), pp. 100091.*

[36] *H. I. Mohammed, F. L. Rashid, H. Togun, E. B. Agyekum, A. Ameen, K. A. Hammoodi, R. Parveen, S. A. Kadhim, and W. N. Abbas, "The role of nanotechnology and artificial intelligence in optimizing thermal energy systems", Applied Energy., vol. 400, (**2025**), pp. 126576.*

[37] *Z. Wei, S. Zhuo, Y. Zhang, L. Wu, X. Gao, S. He, X. Bo, and W. Zhou, "Machine learning reshapes the paradigm of nanomedicine research", Acta Pharmaceutica Sinica B., (**2025**).*

[38] *S. S. Deshmukh and K. S. Yadav, "Next-gen cancer therapy: The convergence of artificial intelligence, nanotechnology, and digital twin", Next Nanotechnology., vol. 8, (**2025**), pp. 100286.*

[39] *A. K. Srivastav and P. Das, Nanobiotechnology: AI and IoT Applications and Emerging Implications, Springer Nature, (**2025**).*

[40] *M. Bhange and D. Telange, "Convergence of nanotechnology and artificial intelligence in the fight against liver cancer: A comprehensive review", Discover Oncology., vol. 16, no. 1, (**2025**), pp. 77.*

[41] *A. B. Mundada, P. Pradhan, R. Raju, Y. S. Sujitha, P. A. Kulkarni, P. A. Mundada, R. Tiwari, and P. Sharma, "Molecular dynamics in pharmaceutical nanotechnology: Simulating interactions and advancing applications", Journal of Biomaterials Science, Polymer Edition., (**2025**), pp. 1–27.*