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Review Article

ADVANCED FABRICATION AND CHARACTERIZATION OF SILVER NANOPARTICLES USING AI TECHNIQUES

ZAINAB LAFI[1,2*], SINA MATALQAH[1,2], SHERINE ASHA[3], NISREEN ASHA[4], HALA MHAIDAT[5], SARA YOUSEF ASHA[3]

[1]Pharmacological and Diagnostic Research Center, Faculty of Pharmacy, Al-Ahliyya Amman University-Amman, Jordan. [2]Department of Pharmaceutics and Pharmaceutical Technology, Faculty of Pharmacy, Al-Ahliyya Amman University-Amman, Jordan. [3]School of Medicine, University of Jordan-Amman. [4]The University of Oklahoma Health Sciences, United States-Oklahoma. [5]King Abdullah University Hospital – Irbid, Jordan

[*]Corresponding author: Zainab Lafi; [*]Email: z.lafi@ammanu.edu.jo

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ABSTRACT

The integration of machine learning (ML) into nanoscience has transformed the fabrication and characterization of silver nanoparticles (AgNPs), enabling precise control over particle size, shape, and functionalization. This review highlights the application of supervised and unsupervised ML models, such as artificial neural networks (ANNs), support vector machines (SVMs), and decision trees, in optimizing AgNP synthesis parameters, including temperature, pH, and reducing agent concentration. Emphasis is placed on green synthesis methods using plant extracts, where ML predicts eco-friendly conditions with minimal experimental input. Characterization techniques benefit from ML-driven image and spectral data analysis, enhancing speed and accuracy. ML is also pivotal in predicting the toxicity and biocompatibility of AgNPs, reducing reliance on animal testing and enabling safer biomedical applications. ML reduced synthesis optimization time by 30%," and to specify the types of ML techniques applied, like neural networks or support vector machines (SVMs). Furthermore, ML enhances functionalization strategies for drug delivery, biosensing, and environmental remediation. By quantifying performance outcomes and improving reproducibility, ML supports the scalable and sustainable development of AgNPs. This review offers a detailed synthesis of current advances and identifies future opportunities for intelligent, data-driven nanomaterial design.

Keywords: Silver nanoparticles, Machine learning, Green synthesis, Toxicity prediction, Artificial neural networks, Support vector machines, Functionalization, Nanomedicine, Biosensors

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INTRODUCTION

Silver nanoparticles (AgNPs) are a notable category of an extensive variety of nanoparticles that have attracted much attention in scientific research owing to their distinctive physical, chemical, and biological properties due to their high surface area and quantum effects [1]. These nanoparticles exhibit strong antimicrobial, conductive, and catalytic properties, making them valuable across various fields, such as engineering, medicine, chemistry, and physics.

AgNPs are extensively utilized in the medical field owing to their antimicrobial characteristics, which make them effective in wound dressing [2], coatings for medical instruments [3, 4], and antibacterial formulations [5, 6]. Additionally, they are being investigated for their potential in cancer therapy [7-9], and drug delivery is attributed to their capacity to selectively target cells [10-12].

AgNPs have been applied in the field of electronics, particularly in conductive inks utilized for printed electronics [13], sensors [14], and flexible circuits. The exceptional conductivity of these materials renders them highly suitable for incorporation into advanced electronic devices [15].

Additionally, AgNPs play a significant role in environmental applications, particularly in the purification of water, owing to their effectiveness in eliminating harmful bacteria and pathogens [16, 17]. Additionally, they contribute to pollution management and the treatment of wastewater by facilitating the degradation of pollutants [18].

The emergence of machine learning (ML) has significantly revolutionized scientific inquiry across various fields, including biology [19], physics [20], chemistry [21], medicine, and the social sciences. ML, which is a branch of artificial intelligence (AI), allows computers to identify patterns within data and to make predictions or decisions autonomously without the need for explicit programming (table 1) [22]. Its transformative impact on scientific research can be understood through several principal domains:

Table 1: Impact of using machine learning (ML) in parameters optimization of $AgNO_3$-based nanoparticle synthesis

Parameter	Range/levels	Impact on outcome	ML optimization approach	Potential algorithms
$AgNO_3$ Concentration	0.1–1.0 M	Controls nanoparticle size and yield	Regression, Classification	SVR, Random Forest, ANN
Reducing Agent Type	$NaBH_4$, AA, etc.	Affects reduction rate and morphology	Categorical Feature Encoding	Decision Trees, SVM
Reducing Agent Conc.	0.1–10 mmol	Influences shape and size distribution	Hyperparameter Tuning	Bayesian Optimization
pH	3–12	Governs nucleation and growth kinetics	Response Surface Modeling	Gaussian Process
Reaction Time	5–120 min	Determines growth completion	Time-Series Prediction	LSTM, ARIMA
Temperature	25–90 °C	Control of reaction kinetics	Regression	XGBoost, ANN
Stabilizer Type	PVP, CTAB, etc.	Affects aggregation and stability	Feature Selection	Random Forest, SVM
Stirring Speed	100–1000 rpm	Influences homogeneity	Optimization via DOE+ML	Genetic Algorithm, ANN
Precursor-to-Reducing Agent Ratio	1:1 – 1:10	Affects size distribution and yield	Multi-Objective Optimization	Evolutionary Algorithms

ML is a particularly expert at processing extensive datasets, revealing patterns that may be challenging or unfeasible for humans to identify through manual analysis [23]. With scientific research producing a growing volume of data from experiments, simulations,

and observations such as genomic information, climate models, and astronomical data, ML algorithms have become crucial for discovering secret insights.

For example, in genomics, ML helps identify patterns in DNA that correspond to diseases or traits [24]; in astronomy, ML is used to classify stars and galaxies from telescope data [25], while in chemistry, ML aids in the discovery of new materials and drug compounds by predicting molecular properties [26].

ML can also be employed to speed up hypothesis testing [27]. Traditionally, scientific research follows a hypothesis-driven approach, wherein a researcher develops a hypothesis and subsequently creates experiments to evaluate it. However, ML facilitates the transition to a data-driven scientific approach wherein hypotheses are derived from initial data analysis. ML models can propose research directions by identifying correlations and patterns within existing datasets, thereby resulting in innovative hypotheses (table 2) [28].

Table 2: Examples of machine learning assisted AgNPs fabrication and optimization

Type of Ag NPs	Reducing agent	Method	Parameter	Application	ML techniques used	Reference
Monodisperse Spherical	Trisodium citrate dihydrate (TSC)	High-throughput microfluidic platform	Nanoparticles with the desired absorbance spectrum.	Relationship between chemical composition and optical properties	DNN BO	[29]
Spherical	Sodium citrate	Ultrasound-intensified Lee-Meisel	Ag: citrate ratio Ultrasound power Reaction	NA	Decision Tree Regressor	[30]
Face-centered cubic	Using soluble starches	Green method	Size temperature, Starch stabilizer $AgNO_3$ concentration	NA	CNN-LSTM hybrid model with accuracy achieved 83.50% of recall.	[31]
Spherical	Sodium citrate	High-throughput synthesis	Concentrations of $AgNO_3$ and citrate Reaction conditions	Ooptical properties absorption spectrum	Nonlinear support vector regression	[32]
Spherical	Tannic acid in the presence of trisodium citrate	Continuous flow T-junction device	Temperature, pH, time	NA	DT, RF, XG Boost	[33]
Polyvinylpyrrolidone coated AgNPs with three Sizes	Variable	721 datasets	Dose, Type, Size Exposure time	Soil enzyme activity	ANN, GA, RF	[34]
Spherical	Titanium citrate and tannic acid	T-junction device	Temperature, Time, chemical Reagent concentration/ratio, Reaction precursors, Reaction ligands, solution reagents, Microreactor channel structure, External stimuli	NA	Tree-based models	[35]

This has led to breakthroughs in fields such as cancer research, neuroscience, automated experimental processes, robotics, autonomous laboratories, predictive modeling and simulation, reducing bias and improving reproducibility and personalized medicine [36-41].

ML plays a transformative role in advancing research on silver nanoparticles (AgNPs), particularly in the areas of synthesis, characterization, functionalization and surface modification; toxicity and biocompatibility; drug delivery and therapeutics; data-driven discovery and design; and, ultimately, environmental role (fig. 1).

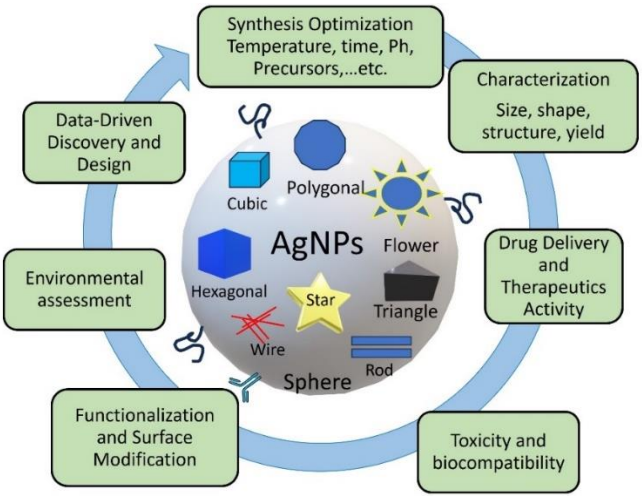

Fig. 1: Different categories for AgNPs fabrication and optimization that need ML integration" while also showing the versatility of AgNPs shapes

In conclusion, the rationale for integrating machine learning (ML) into silver nanoparticle (AgNP) research stems from the inherent limitations of conventional approaches, which often rely on trial-and-error methods. These traditional techniques are not only time-consuming but also resource-intensive, as they typically involve varying one parameter at a time and conducting numerous experimental trials to achieve optimal results. This approach makes it challenging to simultaneously optimize multiple factors and to handle the complexity of the datasets generated. ML, on the other hand, offers a transformative solution by enabling multi-parameter optimization and efficient handling of large, complex datasets [42]. For instance, ML algorithms such as neural networks and support vector machines (SVMs) can learn from existing data to predict optimal synthesis conditions, significantly reducing the time and resources required for experimentation [43]. Additionally, ML can uncover patterns and relationships within the data that are not readily apparent through conventional methods, leading to more precise and reproducible outcomes. The unique suitability of ML for AgNP research lies in its ability to enhance the precision of nanoparticle synthesis, facilitate green synthesis methods, and improve the characterization of nanoparticles through automated analysis of imaging and spectroscopic data [44, 45]. By addressing the limitations of traditional approaches, ML provides a robust framework for advancing AgNP research and development.

Synthesis of silver nanoparticles (AgNPs)

ML has greatly enhanced the synthesis of silver nanoparticles (AgNPs) by increasing the efficiency, accuracy, and characteristics of the materials involved. The primary contributions include the following:

ML algorithms can predict the most suitable synthesis conditions, such as temperature, pH, and concentration, for producing AgNPs of specific sizes, shapes, and characteristics [46]. For instance, these models can determine the optimal combinations of reductants and stabilizers necessary to regulate particle size and morphology effectively.

As the emphasis on environmentally sustainable practices increases, ML plays a crucial role in optimizing the parameters for the green synthesis of silver nanoparticles (AgNPs) utilizing biological agents, such as plant extracts. The influence of different biological components on the properties of nanoparticles, including their size and surface charge, has been predicted [47].

The integration of ML in automation significantly decreases the requirement for physical experiments. This is achieved through the application of methodologies such as design of experiments (DoE) in conjunction with machine learning [48], which accelerates the optimization of the synthesis process [49]. Núñez, R. N *et al.* optimized a method for the synthesis of AgNPs using gallic acid as a reductant via design of experiment strategies based on the response surface methodologies. Fractional factorial design was used in the screening stage, the Box–Behnken method was employed to model the target responses, and the optimization step was performed using the desirability function. They found that the obtained AgNPs presented continuous improvement in the reproducibility of the photophysical properties between batches compared to the synthesis methods reported in the literature. They revealed that ML integration reduced batch-to-batch variability by 20%. Intra-assays, intermediate precision tests and reproducibility tests were performed and confirmed that the different AgNP batches presented equal optical responses, average sizes and size distributions at the 95% confidence level [49]. Additionally, ML techniques are employed to analyze extensive datasets derived from earlier synthesis experiments, revealing hidden patterns that facilitate the prediction of new synthesis pathways. Machine learning (ML) plays a pivotal role in predicting the efficacy of plant extracts used in the green synthesis of AgNPs [50]. One effective approach involves using decision trees to analyze and correlate specific phytochemicals with the resulting nanoparticle size and shape. Decision trees, a type of supervised learning algorithm, can handle complex datasets by breaking down the data into smaller, more manageable subsets based on decision rules derived from the input features. In the AgNPs synthesis, these input features might include the concentration of various phytochemicals present in the plant extracts, such as flavonoids, terpenoids, and phenolic acids [45]. By training the decision tree model on experimental data, it can learn to predict which combinations and concentrations of these phytochemicals are most likely to produce nanoparticles with desired characteristics. For example, the model might reveal that higher concentrations of certain flavonoids correlate with smaller nanoparticle sizes, while specific terpenoids might influence the shape of the nanoparticles. This predictive capability not only enhances the efficiency of the synthesis process but also provides valuable insights into the underlying mechanisms of green synthesis, enabling researchers to select the most effective plant extracts for producing high-quality AgNPs [45, 51].

Characterization of silver nanoparticles

Characterizing silver nanoparticles (AgNPs) requires assessment of their size, shape, surface area, and distribution, as these factors significantly influence their potential applications. Machine learning (ML) techniques enhance this process by facilitating the application of computer vision and ML in microscopy analysis, which significantly improves the identification, classification, and quantification of nanoparticles within microscopy images, such as those obtained from transmission electron microscopy (TEM) and scanning electron microscopy (SEM). Convolutional neural networks (CNNs), for example, can be trained to automatically identify and measure the dimensions of AgNPs in TEM images, reducing the potential for human error and speeding up the characterization process [52]. Additionally, ML models trained on experimental datasets can predict the optical, electrical, and catalytic characteristics of AgNPs by analyzing their synthesis parameters and structural attributes. Uthayakumar *et al.* optimized the size of AgNPs using an artificial neural network (ANN) model, achieving an R^2 value of 0.92 for parameter optimization. Response Surface Methodology (RSM) was also employed to conduct statistical analysis to determine the influence of process parameters on the size of the AgNP [46]. Uthayakumar, H. *et al.* optimized the size of AgNPs and evaluated them by using an Artificial Neural Network (ANN) model. Response Surface Methodology (RSM) was also employed to conduct statistical analysis to determine the influence of the process parameters on the size of the AgNPs [47]. ML algorithms facilitate the interpretation of intricate spectroscopic data, such as UV–Vis [53], FTIR, and Raman spectroscopy data, by establishing connections between spectral characteristics and the size, shape, and surface chemistry of nanoparticles [54]. Sahin, F., *et al.* studied the use of an eco-friendly preparation of a surface-enhanced Raman scattering (SERS) substrate for the ML-assisted detection of pesticides in water. The proposed SERS platform was prepared on copy paper by reducing silver salt using the extract of the natural plant *Cedruslibani*. They reported that the ML-assisted detection of pesticides in water using (SERS) prepared by silver nanoparticles achieved an impressive 95% accuracy. This high level of accuracy demonstrates the effectiveness of combining ML with SERS for sensitive and reliable detection of pollutants in water. The fabricated SERS platform was characterized in detail using SEM, energy-dispersive X-ray spectroscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. The highdensity of silver nanoparticles with an average diameter of 41 nm on the surface of the paper enabled the detection of analytes with nanomolar sensitivity. This SERS capability was used to collect Raman signals of four different pesticides in water [54, 55].

Application of silver nanoparticles

The utilization of ML in research extends the implementation of AgNPs to include AgNPs, which are extensively utilized in antimicrobial applications, and ML models can forecast the effectiveness of specific syntheses against different bacterial strains, thereby optimizing nanoparticles for both medical and industrial uses [46].

ML models are employed to forecast the catalytic activity of AgNPs in various chemical reactions, including applications in environmental remediation, such as pollutant degradation, and industrial catalysis. These models can identify correlations between the characteristics of nanoparticles and their reaction efficiency, thereby informing the development of more efficient catalysts (fig. 2) [56, 57].

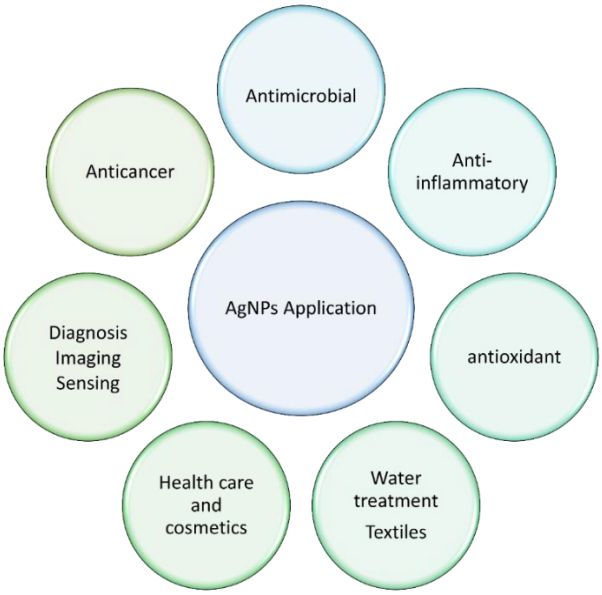

Fig. 2: Illustration scheme of different applications of AgNPs

AgNPs are frequently utilized in biosensors and environmental sensors. ML techniques are employed to improve the sensitivity and specificity of these sensors by forecasting the impact of variations in AgNP size, shape, or surface modifications on their performance [58]. Machine learning (ML) provides a powerful approach for optimizing silver nanoparticle (AgNP) synthesis by analyzing the complex relationships between multiple reaction parameters and their outcomes [59]. Traditional experimental methods rely on trial and error, which can be time-consuming and inefficient. By using ML, researchers can predict optimal conditions for AgNP formation based on historical data, reducing the need for extensive laboratory work [60]. Key factors such as silver nitrate concentration, reducing agent type, pH, temperature, and reaction time significantly influence the size, shape, and stability of AgNPs [61]. ML models, including regression techniques, neural networks, and evolutionary algorithms, can identify patterns and suggest ideal synthesis conditions with high precision. This approach not only improves reproducibility but also accelerates the discovery of novel nanoparticle formulations with tailored properties for specific applications [43]. The integration of ML with real-time monitoring and automation holds great potential for further refining nanoparticle fabrication processes, leading to more efficient and scalable production methods.

Functionalization of silver nanoparticles and surface modification

ML is becoming increasingly important for the functionalization and surface modification of AgNPs. Functionalization involves the attachment of chemical or biological molecules [62, 63] to the surfaces of AgNPs to enhance their characteristics for various applications [46]. Chatterjee *et al.* prepared silver nanoclusters (AgNCs) and silver quantum clusters (AgQCs) via the modification of organic chelating motifs by covalent or noncovalent bonds; these nanoclusters represent an ideal type of hybrid nanomaterial for sensing materials and discussed their applications in metal ions and biomolecule sensing [64]. Similarly, Zhang X *et al.* synthesized hyaluronic acid-coated silver nanoparticles (HA-Ag NPs) that are spherical, ultrasmall and monodisperse and exhibited excellent long-term stability and low cytotoxicity and could be used as a nanoplatform for X-ray computed tomography (CT) and single-photon emission computed tomography (SPECT) imaging after being radiolabeled with ^{99m}Tc [4, 65]. ML contributes to the optimization of these processes by increasing efficiency and precision and facilitating the discovery of innovative functionalization techniques. This process is essential for adjusting the properties of AgNPs, including their stability, biocompatibility, and reactivity. Support vector machines (SVMs) can be used to rank the biocompatibility of various functionalizing agents for silver nanoparticles (AgNPs). This ML model helped in selecting the most appropriate coatings based on predicted biocompatibility, ensuring the nanoparticles were suitable for applications such as imaging and drug delivery [34].

ML has enabled improvements in methods such as the determination of the most appropriate functionalizing agents, such as polymers, proteins, or small molecules, for specific applications [46, 57]. Additionally, ML algorithms are employed to predict the impact of various surface ligands or coatings on the physicochemical characteristics of AgNPs. This approach encompasses the prediction of stability across diverse environments, such as variations in pH and ionic strength, as well as within biological systems such as the bloodstream and tissues. Such predictive capabilities facilitate more precise applications in areas such as drug delivery and biosensing [66]. The surface energy of AgNPs is essential for their interactions with biological cells, other nanoparticles, and solvents. ML aids in optimizing surface modifications to regulate the aggregation, dispersion, and functionalization efficiency of AgNPs [67].

Additionally, ML plays a crucial role in identifying patterns within extensive experimental datasets, facilitating the exploration of novel functionalization strategies [68]. ML tools use extensive datasets to investigate various combinations of surface ligands or polymers that may yield distinctive surface properties. This exploration can result in novel approaches to enhancing the stability, bioavailability, or catalytic efficiency of AgNPs [69]. With the growing emphasis on sustainability, ML plays a crucial role in identifying and enhancing environmentally sustainable functionalization methods. For instance, the application of green functionalization methods using plant extracts or biomolecules can be investigated by employing ML models trained on historical experimental data (fig. 3) [70].

Accurate characterization of functionalized or surface-modified AgNPs is essential for understanding how these modifications impact their behavior in different environments. ML enhances the characterization process by two means: ML techniques, such as computer vision, can be employed to obtain microscopy images (TEM, SEM) of functionalized silver nanoparticles (AgNPs), enabling researchers to efficiently evaluate surface modifications. Similarly, spectroscopy data (e. g., FTIR and Raman) pertaining to surface ligands can be analyzed by ML models to ascertain the extent of functionalization [71]. The other technique is to use ML algorithms that are trained to predict how surface modifications will affect nanoparticle interactions with their surroundings. For example, predictive models can assess how altered AgNPs engage with

proteins in biological contexts or with pollutants in environmental scenarios [72]. ML helps optimize AgNP functionalization for specific applications: AgNPs are widely used for their antimicrobial properties. ML models can predict which surface modifications optimize or refine the antibacterial or antiviral efficacy of AgNPs. For example, these models recommend surface alterations that enhance the interaction with bacterial cell membranes or viral particles [73]. In nanomedicine, the functionalization of AgNPs with ligands or polymers enhances their capacity to selectively target diseased cells, such as cancer cells. ML plays a crucial role in predicting which surface modifications optimize cellular uptake, minimize toxicity, or facilitate drug release at the intended site [74].

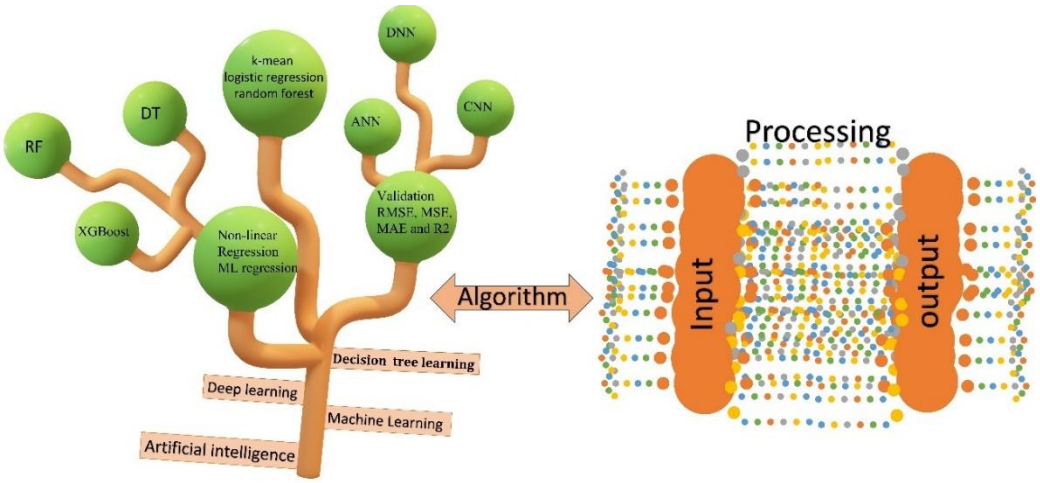

Fig. 3: Illustration scheme of different ML types used in AgNPs good formulation prediction

Surface-modified AgNPs are used in catalysis, particularly in environmental and industrial applications. ML models are used to predict which functionalization approaches will enhance catalytic efficiency, including enhancing reaction selectivity or minimizing energy consumption during chemical transformations [75, 76].

Additionally, functionalized AgNPs are frequently employed in the development of biosensors and chemical sensors. ML assists in forecasting the impact of surface modifications on the sensitivity and selectivity of these sensors, thereby informing the design of highly precise sensing platforms [77].

Different ML techniques are employed in functionalization research: models such as decision trees, support vector machines (SVMs), and neural networks are used to predict the best functionalization agents or surface modifiers based on known datasets [78, 79]. Clustering techniques are used to group AgNPs based on their surface properties or performance in specific applications, helping to identify which functionalization methods lead to similar outcomes [80]. On the other hand, reinforcement learning helps optimize surface modification protocols by dynamically adjusting experimental conditions based on feedback from early experiments, and deep learning is useful for analyzing complex data such as microscopy images or spectroscopic signals [81].

Prediction of silver nanoparticle toxicity

The prediction of AgNP toxicity using ML approaches is a developing area in which data-driven models are utilized to evaluate the potential risks of AgNP exposure [82, 62]. ML models can facilitate the prediction of AgNP toxicity (table 3), thereby minimizing the necessity for extensive biological testing by offering toxicity forecasts prior to experimental validation [83].

Table 3: Some common ML approaches used in the prediction of silver nanoparticle toxicity include the following

Machine learning approach	Description	Examples
Supervised Learning	Trained on labelled data to predict toxicity levels of new nanoparticles.	Random Forest, SVMs, Neural Networks [84]
Unsupervised Learning	Clustering methods identify groups of nanoparticles with similar toxicity profiles, even without labels.	K-Means, Hierarchical Clustering [70]
Regression Models	Predict quantitative toxicity endpoints such as IC50, cell viability, or oxidative stress levels.	Various regression techniques [69]
Classification Models	Categorize nanoparticles as toxic or non-toxic based on physicochemical properties.	Decision Trees, SVM, Logistic Regression [85]
Deep Learning	Captures complex relationships in large datasets using neural networks.	Deep Neural Networks (DNNs) [81]

The fundamental characteristics involved in predicting the toxicity of nanoparticles generally encompass physicochemical properties, including particle size, shape, surface area, zeta potential, and aggregation state [86]. Additionally, the chemical composition of nanoparticles, such as surface coatings, ligands, and dopant elements, plays a crucial role [87, 88]. The environmental conditions, such as temperature, pH, ionic strength, and duration of exposure, are also significant [89]. Furthermore, biological interactions, including cell type, exposure dose, duration, and specific toxicity biomarkers, are essential considerations. These attributes are utilized to train models that establish correlations between the properties of nanoparticles and their toxic outcomes [48].

The application of ML in forecasting the toxicity of AgNPs has several advantages. This approach facilitates the swift evaluation of the toxicological effects of novel nanoparticles, thereby minimizing both time and financial expenditure [90]. Validation metrics, for example, stating that "ANN models achieved 85% accuracy in predicting *in vivo* toxicity." Furthermore, using interpretability tools like SHAP (SHapley Additive exPlanations) to provide insights into the factors influencing toxicity predictions, such as identifying particle size as a dominant factor. Additionally, these models possess the ability to reveal intricate correlations between the characteristics of nanoparticles and their biological impacts, which may be challenging to identify using conventional statistical

approaches. Additionally, these ML models reduce the use of animal testing for toxicity assessments.

ML provides a robust array of tools for forecasting the toxicity of AgNPs by synthesizing information from diverse sources and revealing patterns that may not be readily apparent [91]. These models can assist in the safe development of nanomaterials and reduce potential hazards linked to their application in consumer and medical products. Nevertheless, continuous enhancements in data quality, model interpretability, and generalization are crucial for broader implementation.

Challenges and future directions

The combination of ML and AgNP research presents promising prospects but also introduces several challenges [16, 92]. The following is a summary of the challenges faced and potential future directions in this developing area.

High-quality, large datasets are often required for training ML models [93]. However, obtaining reliable and standardized data on the synthesis, properties, and behavior of AgNPs is challenging due to varying experimental conditions [46]. Additionally, experimental results from different laboratories can be difficult to compare due to variability in protocols, particle sizes, surface coatings, and environmental factors [46]. Many datasets contain incomplete or biased information, which can skew ML model predictions [85].

The behavior of AgNPs is influenced by various factors, ranging from atomic interactions to the properties of bulk materials, which complicates the modeling of all pertinent factors. AgNPs exhibit size, shape, and surface-dependent properties [82]. The challenge is to account for this variability in a model that generalizes across a wide range of conditions. Additionally, simulating AgNP interactions at the atomic or molecular level often requires high-performance computing, which may be limited by certain researchers or institutions.

Determining the appropriate features for ML models is essential. In AgNP research, these features could encompass physical characteristics, environmental factors, and biological interactions, which may be challenging to quantify or may interact in nonobvious ways [94]. The development of suitable descriptors that capture the essential physics and chemistry underlying AgNP behaviors is still a growing area of research. Many researchers, as illustrated in table 4, have used data from literature as an input parameter for the ML algorithm to predict the optimum conditions and effectiveness of AgNPs.

Table 4: Examples of data collected from literature and used in machine learning for predicting optimum parameter and therapeutic effects of AgNPs

Type of Ag NPs	Studies used	Parameter	Application	ML techniques used	Reference
AgNPs is developed for the energy of Fermi level	NA	Multi-structure/single-property relationship	Electron Transfer Property	k-mean, logistic regression and random forest	[95]
Spherical, Hexagonal, Rod, Spindle, Disc, Cubic	Different synthesis method of 60 studies	Hydrodynamic size (nm), Zeta potential, Core size (nm), exposure dose (µg/ml)duration, Surface area, Aggregation	Antibacterial	ML algorithms	[96]
Different types	100 studies	Size, Temperature, Starch stabilizer, $AgNO_3$, Concentration, Bacterial concentration	Antibacterial	ML algorithms	[50]
Different types	70 studies	Hydrodynamic size (nm), Zeta potential, Core size (nm), Exposure dose (µg/ml) duration	Antibacterial/ anti-MDR	ML	[55]
Polyvinylpyrrolidone coated AgNPs with three Sizes	721 datasets	Dose, Type, Size, Exposure time	Soil enzyme activity	ANN, GA, RF	[34]
Different types	1315 dataset from 40 studies	Types of cell lines, exposure time, particle size, hydrodynamic diameter, zeta potential, wavelength, concentration, and cell viability	Relationship between the physical parameters of NPs and their cytotoxicity	Decision Tree (DT) and Random Forest (RF)	[97]
Different types	50 studies	Hydrodynamic size, Zeta potential, Core size, Shape, Exposure and duration, Surface area, Aggregation, Coating	Antibacterial Antifungal	Four different machine-learning regression algorithms and validated the models' performance using four metrics, such as RMSE, MSE, MAE and R2	[43]
Different shapes	All AgNPs produced from te year 2004 to 2022	Reactant concentrations, Experimental conditions Physicochemical properties	Antibacterial efficiencies and toxicological profiles	Regression machine learning algorithm	[98]

The future of combining ML with silver AgNP research promises transformative advancements in nanotechnology, with the potential to revolutionize both scientific understanding and practical applications [99, 100]. As the availability of data increases and models become more sophisticated, ML will enable the rapid and accurate prediction of AgNP toxicity, environmental impact, and efficacy under real-world conditions. Multi-omics integration, ecotoxicological models, and hybrid approaches combining ML with physics-based simulations will allow more precise insights into how AgNPs interact with biological systems and ecosystems [101]. Additionally, the development of explainable AI will enhance model interpretability, allowing researchers to understand the underlying mechanisms of nanoparticle toxicity [102]. In the long term, ML-driven personalized risk assessments, automated nanoparticle design, and sustainable manufacturing practices will emerge, minimizing environmental damage and enhancing the safety of nanomaterials across a range of industries, including medicine, electronics, and consumer products. Finally, implementing FAIR (Findable, Accessible, Interoperable, and Reusable) data principles is crucial to ensure high-quality, standardized datasets for training ML models. Leveraging cloud computing resources can effectively handle the computational demands of simulating AgNP interactions and processing large datasets. Additionally, utilizing synthetic data generation techniques helps balance datasets, address data scarcity,

and improve model robustness [103, 104]. Future research should focus on integrating explainable AI techniques, such as LIME (Local Interpretable Model-agnostic Explanations), to enhance the transparency and interpretability of ML models used in AgNP research. Additionally, the development of ML-DFT (Density Functional Theory) hybrid models can provide more accurate predictions by combining the strengths of machine learning and quantum mechanical simulations. To support collaborative research and reproducibility, establishing open-source repositories for sharing datasets, models, and code is essential [76].

CONCLUSION

Integrating machine learning with silver nanoparticle research holds tremendous promise for advancing our understanding and application of these materials. However, addressing challenges such as data quality, model interpretability, and interdisciplinary collaboration will be key to realizing the full potential of this approach. Future advancements in explainable AI, high-throughput data generation, and hybrid modeling techniques will further enhance the capabilities of ML in nanoscience.

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AUTHORS CONTRIBUTIONS

Zainab Lafi[1*], Idea, Writing about Silver nanoparticles, Drawing, editing and validation

Sina Matalqah[1], Writing about Silver nanoparticles, editing and validation

Sherine Asha[2], Writing drafts about machine learning and constructing tables

Hala Mhaidat[3], Writing drafts about machine learning and constructing tables

Nisreen Asha[4], Writing drafts about machine learning and drawing images

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CONFLICT OF INTERESTS

Declared none

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