
7 Machine Learning Applications for Nano-synthesized Materials Production and Utilization

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7.1 INTRODUCTION

Although there is no internationally accepted definition of a nanomaterial, a material is considered nano if at least one of its dimensions falls within the range of 1–100 nm. By altering the form and size at the nanoscale level, nanomaterials take on distinctive characteristics that differ from their bulk material counterparts, boasting new features and capabilities that make them of significant scientific interest. Because of the changes in size and morphology of the nanomaterials compared to the bulk materials, several unique properties are observed. These properties differ from those of the bulk materials and include aspects such as surface area, thermal effects, thermal and electrical conductivity, mechanical qualities, catalyst support, antimicrobial activities, and magnetism [1]. Because of these unique properties, nanomaterials provide significant advantages in cost, performance, and activity over traditional materials. They are widely employed in various fields including catalysis, agricultural and food production, hydrogen production and storage, construction, and more [2, 3]. These materials can be distinctly classified according to their size, characteristics, and constituents. The classifications include carbon-based nanomaterials, metal nanoparticles, nanoporous materials, ultrathin 2-dimensional nanomaterials, and core-shell nanoparticles [4]. Table 7.1 describes the different types of nanomaterials and their applications in different industries.

Nanomaterials can be synthesized through two main approaches. The first involves using crushing, milling, and grinding procedures to break down bulk materials into smaller particles to create nanostructured materials [16]. The second utilizes methods such as self-assembly or coprecipitation to assemble tiny particles into nanomaterials. These methods include techniques like milling, electrospinning, chemical vapor deposition, hydrothermal synthesis, and green synthesis. Among all the methods of nanomaterial synthesis, green synthesis is considered to be the most environmentally friendly. It offers many potential applications in biomedical and environmental fields and can also eliminate many hazardous properties by enabling

TABLE 7.1**Types of nanomaterials and their applications in different industries**

Nanomaterial Types	Examples	Applications	References
Carbon-based nanomaterials	Fullerenes	Drug delivery tool, transfection agent, and theranostic nanomaterial	[5]
	Carbon nanotubes (CNT)	Artificial implants, genetic engineering, and drug delivery	[6]
	Graphene	Targeted drug delivery, energy storage devices, and electrochemical sensors	[7]
	Nanodiamonds	Bioimaging, drug delivery, and biosensing	[8]
	Quantum dots	LED display, energy conversion, and bioimaging	[9]
Nanoporous materials	Nanocones	Suitable replacement for CNT	[10]
	Activated carbon, porous silicas and zeolins	Energy storage and conversion in fuel cells, solar cells, hydrogen storage and supercapacitors, catalysis, and gas purification	[11]
2-dimensional ultrathin nanomaterials	Sillicene	Quantum sensing and energy devices	[12]
	Mxenex	Energy storage, energy conversion, sensing, optoelectronic, and optical devices	[13]
Metal nanostructured material	Submicron-scale pure metals or their compounds	Catalysis, sensors, optics, and protective coatings	[14]
Core-shell nanoparticles	Ag@Si, Cu@Si, Cu@Ni etc.	Biomedicine, electrical and semiconducting materials, and catalysts	[15]

nanoparticles to be synthesized at lower temperatures, pH, and pressure, all at a significantly reduced cost [17]. The different methods of nanomaterial synthesis are presented in Figure 7.1.

Even with the advancements in nanomaterial synthesis and their growing applications across various industries, there remain ongoing concerns regarding the prediction of nanomaterials' physicochemical properties and the optimization of their production methods. Data-driven machine learning approaches have been introduced to tackle these issues. This chapter provides an overview of several machine learning (ML) models – such as artificial neural networks (ANN), support vector machines (SVM), decision trees, convolutional neural networks (CNN), and deep neural networks (DNN) – that have been used successfully to predict different nanomaterial properties based on experimental data. A detailed examination of these models is included, outlining how they are employed to forecast the physicochemical attributes of nanomaterials. The chapter also discusses the current challenges in utilizing these ML tools and explores the necessary changes for machine learning to have a substantial impact on the field of nanomaterial synthesis in the near future.

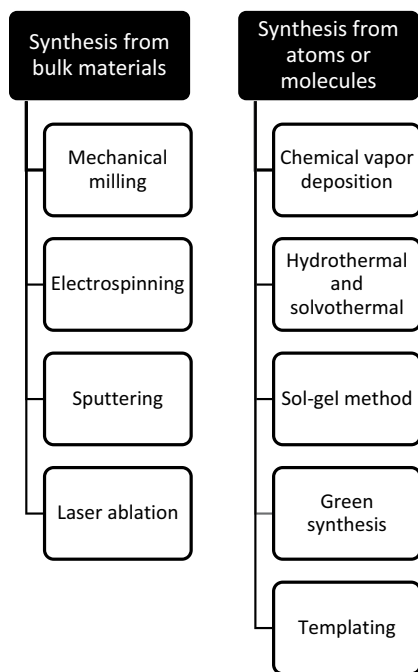


FIGURE 7.1 Different nanomaterial synthesis methods.

(Adapted from [1, 16]).

7.2 MACHINE LEARNING IN NANOMATERIALS

Machine learning (ML) has been applied across various disciplines, making significant contributions to their development. In the realm of nanotechnology, ML has been instrumental in achieving success in predicting properties, optimizing nanomaterial synthesis, and discovering new nanomaterials. The advancements in artificial intelligence have enabled the synthesis and analysis of materials at a pace far exceeding that of traditional one-at-a-time tests, propelling the growth in nanotechnologies. Various ML approaches, including ANN, SVM, decision trees, Gaussian process regression (GPR), Bayesian optimization, convolutional neural networks (CNN), and generative adversarial networks (GAN), have been applied specifically to nanomaterials for property prediction and material discovery [18, 19].

7.2.1 TRADITIONAL ML METHOD IN NANOMATERIALS SYNTHESIS

Traditional ML approaches, which include linear and non-linear regression, ANNs, and decision trees, have been utilized to develop most models of the biological characteristics of nanomaterials [20]. In this section, these approaches will be discussed at length, beginning with an exploration of both linear and non-linear regression techniques.

7.2.1.1 Linear and Non-linear Regression

Linear regression is one of the simplest, yet most powerful statistical methods used to model the relationship between a dependent variable and one or more independent variables. In the context of nanomaterials, it may be applied to predict a biological characteristic based on various physicochemical properties, assuming a linear relationship between them [20]. Unlike linear regression, non-linear regression does not assume a linear relationship between the dependent and independent variables. It can model more complex relationships, making it suitable for the intricate and multifaceted biological characteristics of nanomaterials. This adaptability allows for more accurate modeling of phenomena that are not strictly linear.

7.2.1.2 Artificial Neural Networks (ANNs)

Artificial neural networks (ANNs) are non-linear data processing methods used in various study fields. The neural network can assess different forms of data, discover patterns linked to input-output relationships in the data, and then predict outputs even for new inputs. The ANN model comprises an input layer, a hidden layer, and an output layer. Each neuron layer is made up of a group of neurons. To make reliable predictions, the number of neurons may be arbitrarily adjusted, and prediction model losses can be avoided by altering the number of neurons and activation function parameters. [21]. The ANN modifies the weights and bias parameters to minimize the mean square error (MSE) of the output function. The MSE is defined by Equation (7.1) [22].

$$\text{MSE} = \sum_{i=1}^n \frac{(x_i - y_i)^2}{n} \quad (7.1)$$

where x_i is the experimental value, y_i is the ANN model's projected value, and n is the number of samples in the dataset.

Among the different applications where ANNs have been deployed, one example is by Orimito et al. [23], who used the ANN tool to determine the relationship between the 3404 input and output data obtained from microreactor-based combinatorial cadmium selenide (CdSe) nanoparticle (NP) synthesis. The input parameters, consisting of reaction temperature, time, amine concentration, Cd concentration, Cd/Se ratio, and type of amine, showed a good relationship with the output parameters, such as particle size, CdSe quantum yield, and photoluminescence quantum yield. The trained data successfully predicted the nanomaterial properties even under new experimental conditions.

This machine learning tool has also been used to predict several other nanomaterial synthesis parameters, such as the diameter of a metallic NP (AgNP), which was produced by green synthesis using cashew gum solution. The variable input conditions such as temperature, time, pH, and concentration of the cashew gum solution were examined [24]. Similarly, ANN was used to predict the role of different synthesis parameters, including the concentration of precursors, pH, and operating temperature, on the shape and size of TiO₂ NP [25]. In essence, various nanomaterials

from different synthesis methods have been analyzed to predict outputs such as production efficiency [26] and thermal conductivity [27], among others, based on different synthesis conditions like temperature, time, and pH. A strong prediction relationship was obtained with a correlation coefficient greater than 0.9.

7.2.1.3 Support Vector Machines (SVMs)

Like ANNs, support vector machines (SVMs) are also utilized for regression, classification, and optimization problems especially in the field of nanomaterials. Classification is effectively performed using the kernel approach, which implicitly translates a sample's original feature set into a higher-dimensional feature space. A new sample is categorized based on which side of the margin it falls on [28]. The objective of the SVM model algorithm is to ensure that the projected regression model, given by $(f(x) = wx + b)$, falls within the required accuracy of the experimental output [29].

The SVM tool has been utilized in various nanomaterial syntheses, such as determining the dye removal ability of nanostructured adsorbent (MnO_2) [30], predicting the toxic levels of several nanomaterials [31], and assessing the crystallization level of metal-organic nano capsules [32]. Based on this analysis, the SVM has proven to be a powerful tool for predicting different nanomaterial characteristics.

However, while the SVM is more promising than the ANN in terms of generalization performance on unseen data, its main downside is its “black box” nature. A SVM learns information as a set of numerical parameters, making it challenging to understand what the SVM is actually calculating. The development of new models or the addition of interpretable components to existing models would enhance the interpretability of the SVM in ML [33].

7.2.1.4 Decision Tree

Another ML classification tool used in nanomaterial synthesis is the decision tree. The decision tree is trained to draw links between experimental variables and structural attributes that are difficult or impossible to obtain from a small quantity of simulated training data, thereby removing the need for time-consuming correlated electron microscopy [34]. It also gives an explicit graphical depiction of the decision thresholds for each attribute, which significantly improves the interpretation of NP structure-activity models. The decision tree model works by selecting numerous cut points to split the variables in the dataset. Loss functions are computed for both portions of the divided data, and each cut point is compared to the cut point that yields the least loss result. The regression tree model is constructed based on the optimal cut point. The loss function is defined as (Equation 7.2) [22]:

$$\text{Loss}(y, f(x)) = (f(x) - y)^2 \quad (7.2)$$

Several authors have used decision trees to predict the relationship between input variables in the synthesis and characterization of different nanoparticles. The decision tree was used to estimate the size of gold nanorods based on a simple interaction between the resonance energy and linewidth of the localized surface plasmon

resonance as determined by scanning electron microscopy imaging (SEM) [34]. Similarly, the photocatalytic and cytotoxicity of several multicomponent nanomaterials were analyzed using the decision tree model by Mikołajczyk et al. [35]. The authors used a decision stump approach, followed by a regression metaclassifier, to improve the decision stump’s performance. A single descriptor distinguishes each decision stump. The decision tree’s maximum size was set to four, and the size correlates to the number of decision stumps. The contribution of several physicochemical factors (the content of silver vs. gold/palladium/platinum, solubility, the electronic properties of a sample, and photocatalytic activity) on photocatalytic properties and environmental toxicity was obtained based on the developed model and experimental evidence obtained.

A random forest regression, a subset of the decision trees, works on the premise of developing multiple distinct decision trees, each of which may be trained individually given training samples. The approach is built on ensemble learning, which can help prevent specific overfitting issues and provide the model with more generality and accuracy [36].

Using the random forest regression, Mirzaei et al. [37] predicted the antibacterial capacity of several nanoparticles. With over 1000 rows of experimental data obtained from 60 articles, input variables such as type of NP, different nanospecific distributors, bacteria characteristics and exposure conditions were used to predict different anti-bacterial measurements such as bacteria viability, minimum bactericidal concentration and zone of inhibition, amongst others. Compared with other regression analysis (SVM, elastic net regression (ENR), ridge regression (RR) and lasso regression), the random forest had the highest R^2 value and the lowest MSE as seen in Figure 7.2. The random forest also determined which input variable has the most effect on the anti-bacterial capacity, which is the core size from the nano-specific distributor.

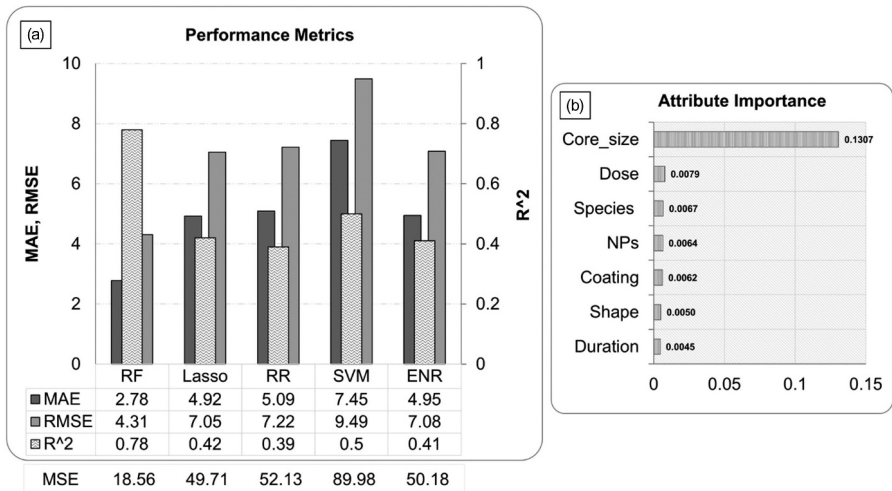


FIGURE 7.2 Performance evaluation of different ML regression analysis models compared with the random forest (RF) [37].

7.2.2 DEEP LEARNING METHODS IN NANOMATERIAL SYNTHESIS

Deep learning approaches use neural networks with more hidden layers and complex architectures with the capacity to identify patterns in images, speech recognition, and dynamic decision making [38]. Deep learning differs from typical machine learning methods in that it employs a hierarchical cascade of non-linear functions. The role of each level is to transform its given data into a conceptual and representation feature that provides input for the succeeding levels. This offers it the comparative benefit of not requiring the scientist to manually conduct feature engineering since the algorithm exhibits self-adjustment efficiency and the ability to identify suitable features independently in a continuous learning process. Convolutional neural networks (CNNs) [39], deep neural networks (DNNs) or autoencoders [40], and generative adversarial networks (GANs) [41] are some of the most extensively used deep learning techniques for nanomaterials synthesis (Figure 7.3).

7.2.2.1 Convolutional Neural Networks (CNN)

A CNN uses several convolutional layers and pooling for complex, multidimensional data. The convolutional layer has a kernel that determines the collected features, and the pooling layer minimizes the number of parameters, lowering the computational complexity even further [19]. Individual neurons which are inside the CNN screens are trained to do mathematical computations and can distinguish tiny, different components of input data that are crucial to a given modeling job. The CNN is mostly

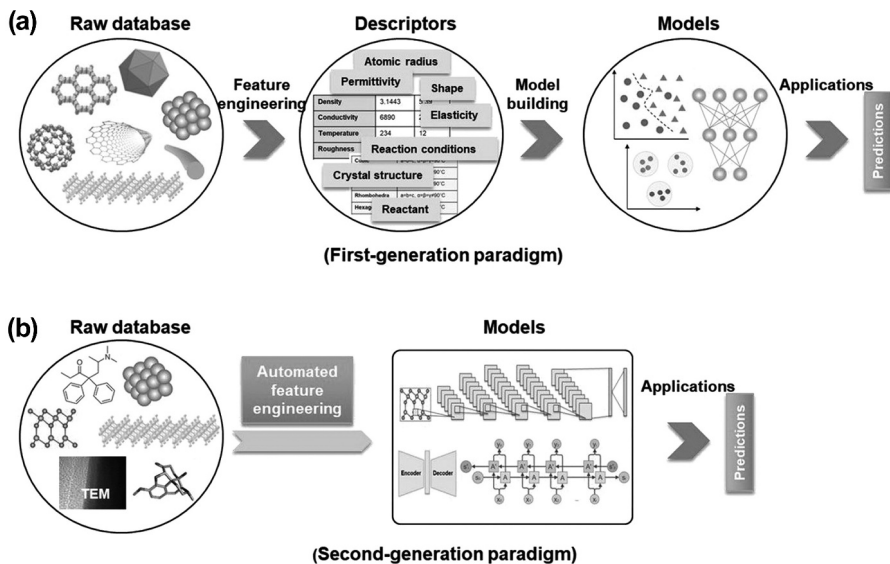


FIGURE 7.3 Difference between the traditional ML (a), and deep learning methods (b). (Copied with permission from Wang et al. [42]).

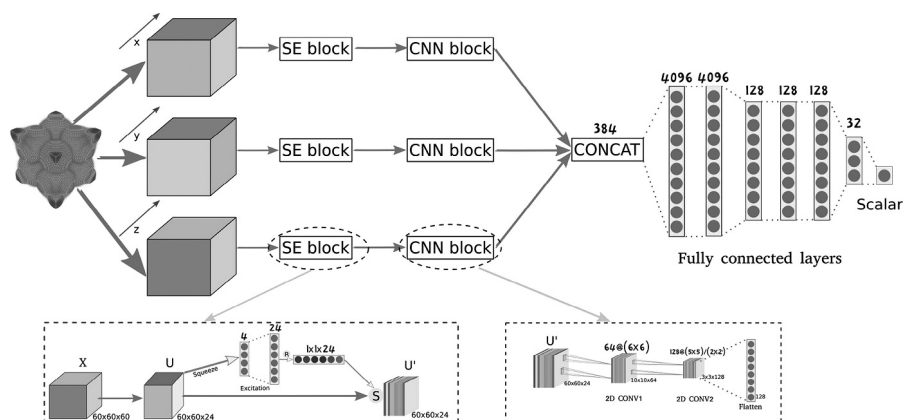


FIGURE 7.4 2D CNN architecture with convolutional, pooling, and fully interconnected layers.

(Reposted with permission from Zhao et al. [45]).

used in nanotechnology to identify nanoparticles in electron microscope pictures (scanning electron microscopy (SEM), signal intensity maps (SIM), transmission electron microscopy (TEM) etc.) [43, 44] (Figure 7.4).

Kolenov et al. [46] used a CNN in classifying and detecting nanoparticles (polystyrene latex nanosphere) deposited in wafers from a SIM. The authors acquired training data from calibrated samples of polystyrene latex (PSL) nanospheres spin-coated on silicon wafers varying in diameter from 40 to 80 nm and investigated the parts of the wafer where the nanoparticle is not present, adding to the “background” class. From the 1302 images given to the network, a dataset with around 260 images per class was constructed, and a 60-20-20 split for training, validation, and testing was implemented. To ensure representative images, the dataset was generated by randomly separating data from each class into three sections and then combining them to generate unbiased sets. The CNN classification method outperformed the traditional ML method for analyzing dispersed maps presented by the authors using modified K-means [47] with an accuracy enhanced by a factor of two for relatively tiny particles with sizes (classes) of 40 and 50 nm.

A CNN was also used for nanostructures in virtual molecular projections [48], spatial distribution maps [49], and TEM images of nanoparticles [43]. This deep learning approach was able to quantitatively analyze a trained CNN with neurons capable of recognizing distinct nanostructure features critical to activities and physicochemical properties, as well as recognizing other nanoscale ordered structures and successfully performing image classification with 94% accuracy. In general, a CNN trained to detect nanoparticles may discover other properties, such as color patches, topography, or backgrounds, that can become highly predictive and be widely employed to design nanoparticles strategically with the desired function.

7.2.2.2 Deep Neural Networks (DNN)

Deep neural networks (DNNs) are composed of two networks: one that maps each material to a result and the other that maps the result to one or more materials. Based on the learned ML model, this deep learning tool, also defined as an autoencoder, may reduce the dimensionality of datasets and forecast materials with specific attributes [41]. A DNN is also helpful for predicting output parameters from input variables when the link between input and output variables is uncertain [50].

The deep learning neural network has been used in several nanomaterials' applications. Amor et al. [51] used the DNN to predict the dye removal ability of nano TiO₂ by mapping out the input-output relationship in order to obtain an optimum result. The input variables consist of the chemicals used in synthesizing the nano TiO₂ and the reaction time. At the same time, the output was the dye-removal efficiency obtained by evaluating the discoloration of methylene blue solution under UV light. An R² value greater than 0.99 was obtained with a non-linear relationship between the input and output conditions.

Interestingly, DNN was used to predict the biological fate of gold (Au) NP (spleen and liver accumulation of AuNP) when the nanoparticle was injected into the bloodstream [52]. The dataset included 63,630 proteins' label-free quantitative (LFQ) intensities and five different Au nanoparticle sizes (8–80 nm) which were the input parameters and quantified Au in the blood for over 24 hours & gold content in the liver and spleen that serves as the output. The deep learning model predicted the injected nanoparticle size with over 90% accuracy, liver accumulation with 81%–93% accuracy, spleen uptake with 77%–92.6% accuracy, blood half-life of nanoparticles with 84%–91% accuracy, and biological fate with 77%–94% accuracy.

7.2.2.3 Generative Adversarial Networks (GANs)

Generative Adversarial Networks (GANs) were employed to create nanophotonic structures with exact user-defined spectrum responses. A GAN comprises two parts: a generator that creates trial structure-property models and a discriminator that compares the quality of trial models to existing unlabeled data [53]. Just like DNNs, GANs can also convert structural, physicochemical, and processing parameters in nanomaterials into latent variables/descriptors that may be utilized to create ML models of attributes crucial to the utility and safety of nanomaterials.

Although a GAN has not been individually used in nanomaterial synthesis and application, it has been combined with a CNN to create nanophotonic antennas that are not limited by specified designs [54].

7.3 CHALLENGES AND FUTURE OUTLOOK

Although machine learning has the ability to make predictions with minimum human input and significant time and performance efficiency, it also introduces new hurdles in ensuring forecast accuracy in nanomaterials research. Several challenges have been presented by Brown et al. [41] which include a shortage of datasets that are not constrained to the parameter space of the target issue, fluctuating ML performance owing to the use of simulation data for data training instead of experimental data

since it is faster, and difficulties integrating and harmonizing datasets. Apart from the issues of data sets, problems with descriptors are also present for machine learning potentials, particularly for materials with complicated chemical compositions. Because of the necessity for a considerable number of data sets and rising descriptors, training machine learning potentials is exceedingly tough, complicated, time-consuming, and expensive [19].

Furthermore, guaranteeing model performance is crucial because only relevant characteristics are helpful for the creation of prediction models [55]. However, due to the requirements of deep insight into both domain-expert knowledge and the implementation of learning algorithms, selecting the most relevant features is somewhat tricky.

In order to solve the challenge of shortage of datasets, Hiszpanski et al. [56] produced scientific article-processing tools that capture and organize information from nanomaterials publications' text and images, allowing the establishment of a customized knowledge base for nanomaterials synthesis that can be mined to help inform future nanomaterials research. This was accomplished by: (1) creating a relevant corpus of nanomaterials articles, (2) extracting metadata from each article, (3) processing the text of each article to identify the target nanomaterial's morphology and composition, and (4) extracting and further processing SEM/TEM figures of nanomaterials to obtain their morphology and size distributions. This tool has the potential to speed up the discovery of novel nanomaterials. In the future, large nanomaterials databases, such as PubChem or protein data bank (PDB) format, can be used to facilitate rational nanomaterial design and the establishment of data-driven structure-activity relationships, as well as safety, ethics, and regulatory compliance [57].

Also, ML model combinations can be used to swiftly predict the functional parameters of hypothetical NMs at a resolution unattainable by computational or experimental approaches, as well as to discover principles or rules that could govern rational NM and also to detect interior flaws in three-dimensional NMs using computed tomography (CT) images [33].

Finally, future advances in data generation for nanomaterial synthesis via machine learning will guarantee that various scientific and socioeconomic information is combined to detect trends and requirements for society on time and optimize the commercialization benefits of nanotechnology.

7.4 CONCLUSION

Due to the rapid development and synthesis of nanomaterials, faster exploration and characterization of nanomaterials is inevitable. This chapter described several ML tools that have successfully predicted the properties of nanomaterials based on different input properties used in their synthesis. The use of ANNs, SVMs, decision trees, CNNs, and DNNs and the problems associated with their use were all described in detail. Prospective thoughts on changes that must occur in the near future in order to make a more meaningful contribution to nanomaterial synthesis were also presented. Through the aid of ML tools, the development of safe nanomaterials for industrial applications can be expedited with high accuracy.

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