

Review

Intelligent Algorithms Enable Photocatalyst Design and Performance Prediction

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Abstract: Photocatalysts have made great contributions to the degradation of pollutants to achieve environmental purification. The traditional method of developing new photocatalysts is to design and perform a large number of experiments to continuously try to obtain efficient photocatalysts that can degrade pollutants, which is time-consuming, costly, and does not necessarily achieve the best performance of the photocatalyst. The rapid development of photocatalysis has been accelerated by the rapid development of artificial intelligence. Intelligent algorithms can be utilized to design photocatalysts and predict photocatalytic performance, resulting in a reduction in development time and the cost of new catalysts. In this paper, the intelligent algorithms for photocatalyst design and photocatalytic performance prediction are reviewed, especially the artificial neural network model and the model optimized by an intelligent algorithm. A detailed discussion is given on the advantages and disadvantages of the neural network model, as well as its application in photocatalysis optimized by intelligent algorithms. The use of intelligent algorithms in photocatalysis is challenging and long term due to the lack of suitable neural network models for predicting the photocatalytic performance of photocatalysts. The prediction of photocatalytic performance of photocatalysts can be aided by the combination of various intelligent optimization algorithms and neural network models, but it is only useful in the early stages. Intelligent algorithms can be used to design photocatalysts and predict their photocatalytic performance, which is a promising technology.



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1. Introduction

The rapid development of global science and technology has resulted in the gradual application of neural network models to chemical synthesis, material design, and the discovery of efficient catalysts. According to Refs. [1–4], rapid economic development has a negative impact on the global environment, resulting in countries around the world investing a lot of labor and material resources in designing new catalysts to reduce environmental pollution [5–11]. In the early stage of the development of photocatalysts, it is only through constantly preparing different catalysts and conducting photocatalytic experiments that effective photocatalysts can be found [12,13]. The unremitting efforts of scientists from various countries have resulted in the development of numerous photocatalysts with different catalytic activities [14–19]. Researchers have created many new heterojunction composite photocatalysts due to the low photocatalytic activity of a single-component photocatalyst and its inability to meet special needs like magnetic separation [20–25]. However, the development of these photocatalysts is a trial-and-error method, which requires a large number of experiments as support, and most of them rely on luck to synthesize photocatalysts with

efficient photocatalytic activity, which greatly limits the research and development of new photocatalysts [26–32].

With the rapid development of artificial intelligence, new photocatalysts are being introduced to meet the increasing market demand [33,34]. The development of neural network models has led to a surge in research into developing new efficient photocatalysts [35,36]. The use of neural network models is widespread in the synthesis of new photocatalysts, the prediction of catalytic activity of photocatalysts, and the prediction of energy band values of photocatalysts based on first principles [37–39]. Despite the widespread use of neural networks to study novel photocatalysts, neural network models require a significant amount of experimental or theoretical data to accurately predict the photocatalytic activity of photocatalysts or to develop novel photocatalysts [40]. While there are numerous publications on the photocatalytic activity of photocatalysts, the environmental parameters discussed are not consistent, including light source, irradiation power, catalyst content, pollutant concentration, pH value, reaction solution temperature, and other variables. The use of different testing equipment by different research groups results in different test results. Different experimental parameters are chosen by researchers depending on their habits. The training of neural network models requires the use of experimental data of various scales, making it very difficult and challenging.

To solve these problems, researchers have worked hard to create a number of standard databases so that computational scientists will not encounter these difficulties when using data to obtain effective neural network models [41,42]. These standard databases include the Inorganic Crystal Structure Database (ICSD), Crystallography Open Database (COD), Citration, Materials Project (MP), and National Solar Radiation Database (NREL), among others [41,42]. The technology of designing new photocatalysts based on the crystal structure, cell parameters, cell volume, and energy band value calculated from first principles has been relatively mature [43,44]. However, it is difficult to evaluate the photocatalytic activity of photocatalysts using different environmental parameters. How to integrate the data from different research groups and different devices will be the biggest challenge. At present, most research centers on evaluating and predicting the photocatalytic activity of these catalysts according to different catalysts or environmental parameters. The development of the industry can be guided by jointly designing novel photocatalysts, establishing effective neural network models, and predicting their catalytic activity through cooperation between different research groups.

In this review article, we analyze the process of using machine learning in photocatalyst research, from data collection to the establishment of an intelligent algorithm model and the realization of photocatalyst design. Simultaneously, we reviewed the application of all intelligent algorithm-optimized neural network models in predicting the photocatalytic activity of photocatalysts, providing a technical reference for the subsequent development of new intelligent algorithm-optimized neural network models to predict the photocatalytic activity of photocatalysts. By selecting the appropriate neural network model and constructing the corresponding algorithm model, the photocatalytic activity of the photocatalyst can be effectively predicted. Intelligent algorithm-optimized neural networks have also been used to develop new photocatalysts, predict the photocatalytic activity of photocatalysts, and predict the absorbance curves of pollutants with different irradiation times obtained during the photocatalysis process. The neural network model has its own application range and limitations that require improvement or optimization. This paper also discusses different intelligent algorithms to optimize the neural network model and predict the photocatalytic activity of photocatalysts. Based on the current research direction and development trend, the future research work of intelligent algorithms in the field of photocatalyst design is discussed.

2. The Processes of Intelligent Algorithms Design Photocatalysts or Predict the Photocatalytic Activity

The design of new photocatalysts by machine learning mainly depends on the phase structure, microstructure, and other crystallographic data of the photocatalyst itself. Three methods can be employed to obtain these data. (1) Search through the existing database to obtain the corresponding data. (2) Data under various environmental parameters was collected from the literature. (3) Perform relevant experiments to obtain the corresponding experimental data. For theoretical computing researchers, the effective way to obtain data is mainly through the first two. In addition to some of the databases mentioned above, there are also the International Union of Crystallography, Cambridge Structural Database, Open Catalyst 2020, International Centre for Diffraction Data, National Institute of Standard Technology, Open Quantum Materials Database, and NIMS Materials Database [41,42]. The literature mainly includes research papers, conference papers, books, patents, and other image materials. Figure 1 displays the flow chart of an intelligent algorithm predicting the photocatalytic performance of the photocatalysts.

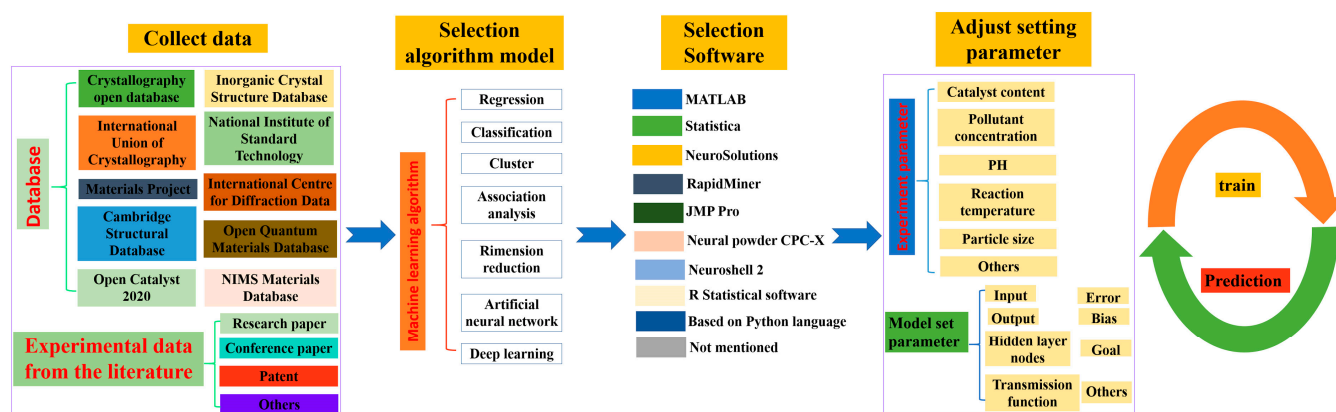


Figure 1. Flow chart of intelligent algorithm predicting photocatalytic performance of the photocatalysts.

The machine learning algorithm will determine the appropriate algorithm model for calculation after collecting the data. There are many machine learning algorithms, including regression, classification, clustering, association analysis, dimension reduction, artificial neural networks, and deep learning. Different data are suitable for different algorithm models, and, with the development of science and technology, these models are constantly evolving to make the collected data suitable for new models. According to the different problems to be solved and the characteristics of the algorithm model, exploring the complementary advantages of the models is more conducive to the accurate design of the photocatalyst or the prediction of the photocatalytic performance.

According to different algorithm models, many suitable software packages have been developed to process the data. Common software currently consists mostly of MATLAB 2018b, Statistica 8.0, NeuroSolutions V7.0, RapidMiner 5.3.015, JMP Pro 16, Neural powder CPC-X, Neuroshell 2, R Statistical software, software based on Python language, and other software [41,42]. MATLAB provides many modular operation modules, a low threshold for the theoretical knowledge of the algorithm model, and is easy to operate and implement, making it the most popular software for intelligent algorithm learning and prediction. In the field of photocatalyst design and photocatalytic performance prediction, MATLAB has been indispensable in completing its due mission. Software such as Python 2.7 language requires a thorough grasp of the theoretical knowledge of machine learning in order to be able to program easily, and there are certain knowledge reserve requirements for beginners. The market demand continues to grow, resulting in the development of other machine learning programming software. Among these software, MATLAB 2018b is the most popular software, with a usage rate of more than 60%. According to Ref. [45], Statistica software not only provides users with general functions such as statistics, plotting, and data

management programs, but also provides data analysis methods such as neural networks for users to use; the usage rate is almost second only to MATLAB software. The use of related software is relatively small, but a large proportion is due to the requirement for a strong background in neural network theory in Python-programmed software. Less than 5% is the usage rate for the other software listed in Figure 1.

Upon the determination of the processing software, the appropriate experimental parameters are chosen to be adjusted and set to prepare for training and predicting the photocatalytic performance of the photocatalyst [46,47]. Take the artificial neural network algorithm model as an example and select the appropriate environmental parameters as the model input, such as catalyst content, pollutant concentration, pH, reaction temperature, particle size, and other environmental parameters. Then, set the appropriate input and output parameters according to the environment parameters, and then calculate the number of nodes in the hidden layer, the transmission function, the error, the threshold, the precision, and other setting parameters. Based on the above preparation and parameter setting, the model is trained, and then the photocatalytic performance is predicted using the trained model that meets the error requirements.

3. Neural Network Model

3.1. Neural Network Model Suitable for Photocatalyst Development

For the prediction of photocatalytic activity of photocatalysts, the choice of neural network model is particularly important. Therefore, it is necessary to understand the current development of neural network models, especially their scope of application, advantages, and disadvantages. Neural network models are a group of machine learning algorithms that have developed into numerous applicable models based on the problem they are addressing. The McCulloch–Pitts (MP) model is the first mathematical model of artificial neural networks, which has been abstracted and developed into a finite automaton theory [48]. The perceptron is the actual model that goes from theoretical research to the process realization stage, and it sets off the first peak of artificial neural network research. Subsequently, it evolved into 27 more popular models, including Perceptron (P), Feed Forward (FF), Radial Basis Network (RBF), Deep Feed Forward (DFF), Recurrent Neural Network (RNN), Long/Short-Term Memory (LSTM), Gated Recurrent Unit (GRU), Autoencoder (AE), Variational AE (VAE), Denoising AE (DAE), Sparse AE (SAE), Markov Chain (MC), Hopfield Network (HN), Boltzmann Machine (BM), Restricted BM (RBM), Deep Belief Network (DBN), Deep Convolutional Network (DCN), Deconvolutional Network (DN), Deep Convolutional Inverse Graphics Network (DCIGN), Generative Adversarial Network (GAN), Liquid State Machine (LSM), Extreme Learning Machine (ELM), Echo State Network (ESN), Deep Residual Network (DRN), Kohonen Network (KN), Support Vector Machine (SVM), and Neural Turing Machine (NTM), as shown in Figure 2. Function approximation, data clustering, pattern classification, and optimization calculation can be achieved through the use of these neural network models. Among these models, P, FF, RBF, SVM, and NTM are multi-input single-output models. MC, HN, BM, RBM, and KN are neural network models with no output. All the other models are multiple-input multiple-output models. According to the law that the photocatalytic activity of photocatalysts is affected by environmental parameters such as pH, catalyst content, initial concentration of pollutants, reaction time, reaction temperature, etc., a suitable model is selected for prediction. Due to the influence of computing resources and the number of samples, selecting the appropriate activation function can save the storage space or improve the computing speed. Therefore, the choice of neural network model should be considered in combination with the available computing resources and the original data. Under normal circumstances, it is necessary to normalize the original data, and then perform the anti-normalization processing after the calculation is completed. Currently, the following neural network models have been used to predict the photocatalytic performance of photocatalysts: Perceptron (P), feed forward (FF), radial basis network (RBF), deep feed forward (DFF), recurrent neural network (RNN), long/short term memory (LSTM),

restricted BM (RBM), deep convolutional network (DCN), generative adversarial network (GAN), extreme learning machine (ELM), echo state network (ESN), and support vector machine (SVM) [49–58]. In addition to the models mentioned above, the backpropagation (BP) neural network model is the most popular model for predicting the photocatalytic performance of various photocatalysts [59–61]. To make up for the shortcomings of a single neural network model, it has become a trend to combine multiple neural network models to predict the photocatalytic activity of photocatalysts.

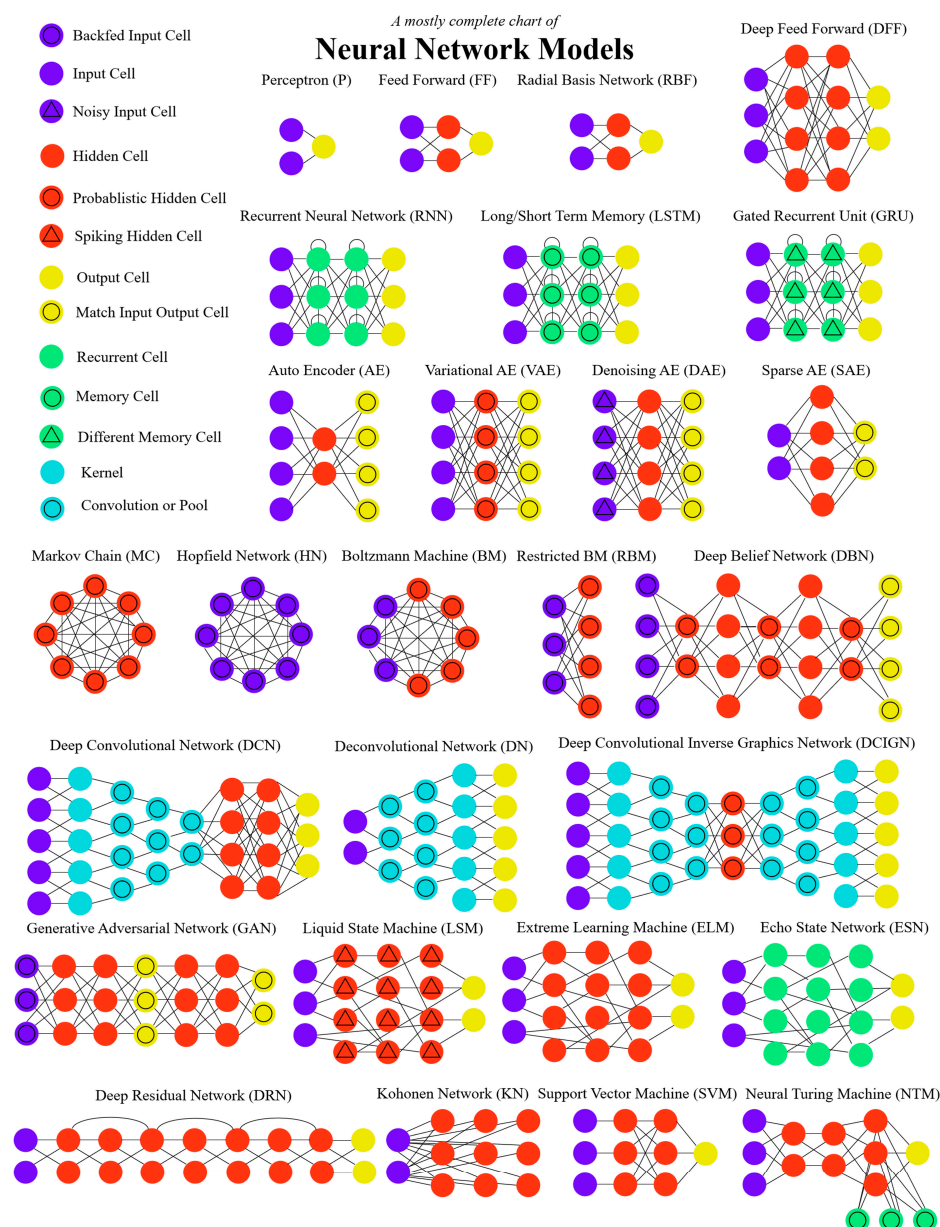


Figure 2. Current development of neural network models (from the network).

3.2. BP Neural Network Model

The basic principle of the BP neural network is the gradient fastest descent method, and its main goal is to adjust the weight to minimize the total error of the network [62]. In the prediction of the photocatalytic performance of photocatalysts, the weights between the input layer and the hidden layer or between the hidden layer and the output layer can be adjusted based on different environmental parameters, and it is easy to obtain an effective training model. Simultaneously, the BP neural network can be applied to information processing, image recognition, model recognition, system control, and so on because of its

excellent ability to approximate nonlinear mapping. The reason why BP neural networks are popular is that they have the following advantages. (1) The connection weights of each layer of the BP network can be adjusted through learning. (2) The basic processing unit of the BP network (except for the input layer) is a nonlinear input–output relationship, and a sigmoid function is generally selected. (3) The BP network can realize the nonlinear mapping relationship between input and output, but it does not depend on the model. (4) The learning algorithm of the BP network is based on the method of global approximation, which means it has good generalization capabilities. For the transfer function between the input layer and the hidden layer, a nonlinear sigmoid transfer function is selected, while the transfer function between the hidden layer and the output layer is a linear transfer function. The formulas for the corresponding sigmoid and linear transfer functions are given in Formulas (1) and (2).

$$\text{tansig}(n) = \frac{2}{1 + e^{-2n}} - 1 \quad (1)$$

$$\text{purelin}(n) = n \quad (2)$$

where n is the net input signal. Since the range of values for the transfer function is $(-1, 1)$ or $(0, 1)$, it is necessary to normalize the data that do not fall within these two ranges before training with MATLAB software. The normalization formulas for the values of the transfer function in $(-1, 1)$ and $(0, 1)$ are Formulas (3) and (4), respectively [63].

$$x_{\text{norm}(-1,1)} = \frac{2X_i}{X_{\max} - X_{\min}} - 1 \quad (3)$$

$$x_{\text{norm}(0,1)} = \frac{X_i - X_{\min}}{X_{\max} - X_{\min}} \quad (4)$$

where $x_{\text{norm}(-1,1)}$ and $x_{\text{norm}(0,1)}$ are the normalized functions, X_i is the experiment value, $X_{\max}$ is the maximum value and $X_{\min}$ is the minimum value. The relative importance (S_s) of input parameters (s) can be estimated by Equation (5) [63].

$$S_s = \frac{\sum_i (\frac{\omega_{sj} u_{jk}}{\sum_i \omega_{ij}})}{\sum_i^m \sum_j^n \sum_k (\frac{\omega_{sj} u_{jk}}{\sum_i \omega_{ij}})} \quad (5)$$

ω_{ij} is the weight value of the input parameter from i to the neuron of j . u_{jk} is the weight value of the neuron from j to the output neuron of k . m is the number of input parameters. n is the number of hidden layers and k is the number of output layers.

The validity of the model is evaluated by the following parameters [64,65]:

$$\text{Correlation coefficient : } R^2 = 1 - \frac{\sum_{i=1}^N (X_{\text{Pred}(i)} - X_{\text{Exp}(i)})^2}{\sum_{i=1}^N (X_{\text{Pred}(i)} - \bar{X}_l)^2} \quad (6)$$

$$\text{Adjusted coefficient of determination : } R_{\text{adj}}^2 = 1 - ((1 - R^2) \frac{N - 1}{N - K - 1}) \quad (7)$$

$$\text{Sum of squares : } SSE = \sum_{i=1}^N (X_{\text{Pred}(i)} - X_{\text{Exp}(i)})^2 \quad (8)$$

$$\text{Sum of the absolute error : } SAE = \frac{1}{N} \sum_{i=1}^N |X_{\text{Pred}(i)} - X_{\text{Exp}(i)}| \quad (9)$$

$$\text{Mean squared error : } MSE = \frac{1}{N} \sum_{i=1}^N (X_{\text{Pred}(i)} - X_{\text{Exp}(i)})^2 \quad (10)$$

$$\text{Root mean square : } RMSE = \sqrt{\frac{\sum_{i=1}^N (X_{\text{Pred}(i)} - X_{\text{Exp}(i)})^2}{N}} \quad (11)$$

$$\text{Absolute average deviation : AAD} = \frac{\sum_{i=1}^N \left| \frac{X_{\text{Pred}(i)} - X_{\text{Exp}(i)}}{X_{\text{Pred}(i)}} \right|}{N} \times 100 \quad (12)$$

$X_{\text{Pred}(i)}$ and $X_{\text{Exp}(i)}$ are the experimental and the predicted values, respectively. The trained model becomes more efficient when R^2 is close to 1 and other parameters are close to 0.

3.3. Limitations of Neural Network Models

Whether the neural network model is suitable for training the existing experimental data mainly depends on the characteristics of the neural network model, the type of data, and whether it can be processed according to the data format required by the neural network model. The model based on the BP neural network has the following shortcomings: (1) the convergence speed of the BP neural network model is slow. (2) The BP neural network model can be easily restricted to local extreme values. (3) The BP neural network model has a difficult time determining the number of hidden layers and nodes. As long as there are enough hidden layers and hidden layer nodes, complex mapping relationships can be realized theoretically. Determining the network's structure based on specific problems is not a good method, and it still requires experience and trial and error. To overcome the shortcomings above, the BP neural network model can be improved by adding an induced-inertia term or an item of momentum to enhance its approximation characteristics and generalization ability of the model. In addition, the neural network model can be optimized by combining other deep learning algorithms such as simulated annealing, genetic algorithm, tabu search, neural network, beetle search algorithm, sparrow search algorithm, dung beetle optimization algorithm, whale algorithm, fuzzy logic, particle swarm optimization algorithm, immune algorithm, distribution estimation algorithm, etc. [66,67]. To obtain an effective training model, it is necessary to overcome the shortcomings of the neural network model.

4. Intelligent Algorithm Optimization of Neural Network Model

Traditional neural network models cannot meet the increasing computing requirements, forcing researchers to combine intelligent optimization algorithms with neural network models to obtain effective prediction models that meet the needs [68–70]. Among many optimization algorithms, only the genetic algorithm, whale algorithm, sparrow search algorithm, and particle swarm optimization algorithm have been used to optimize the neural network model for the prediction of photocatalytic performance of photocatalysts.

4.1. Neural Network Model Optimized by Genetic Algorithm

A genetic algorithm is used to search for the optimal solution by simulating the natural evolutionary process. The algorithm converts the process of solving problems into a process similar to the crossover and variation of chromosome genes in biological evolution using mathematics and computer simulation. When solving complex combinatorial optimization problems, unlike some conventional optimization algorithms, it is usually able to obtain better optimization results faster [71,72]. Taherkhania et al. [73] utilized an optimized neural network model that was developed through a genetic algorithm to predict how much zinc stannate degraded tetracycline hydrochloride (TC). During the training, three different algorithms, including scaled conjugate gradient (SCG), gradient descent (GD), and Levenberg–Marquardt (LM) algorithms were used to train the experimental data. Figure 3 displays the ANN-GA model and prediction process. Input parameters include the initial pH of the reaction solution (pH), photocatalyst dosage (ZTO), initial pollutant concentration (TC concentration), and reaction time (time). The output layer represents the degradation percentage of TC that has been degraded by zinc stannate. The number of nodes in the hidden layer is 20. A total of 65 sets of data were collected, 70% of which were used for training, 15% for confirmation, and 15% for testing. The genetic algorithm's calculation process is carried out after the completion of neural network training. Although the trained model is evidently better than the artificial neural network model optimized by a genetic

algorithm, it requires a longer computation time [73]. The mathematical representation of an artificial neural network model that has been optimized by genetic algorithms is as follows [74]:

$$\text{Max net (pH; ZTO; TC concentration; time)} = \text{TC removal (\%)} \text{ as objective function} \quad (13)$$

$$\text{Bound constraints} \begin{cases} 4.5 \leq \text{pH} \leq 10.5 \\ 100 \leq \text{ZTO dose} \leq 300 \text{ (mg/L)} \\ 10 \leq \text{TC concentration} \leq 30 \text{ (mg/L)} \\ 10 \leq \text{time} \leq 120 \text{ min} \end{cases} \quad (14)$$

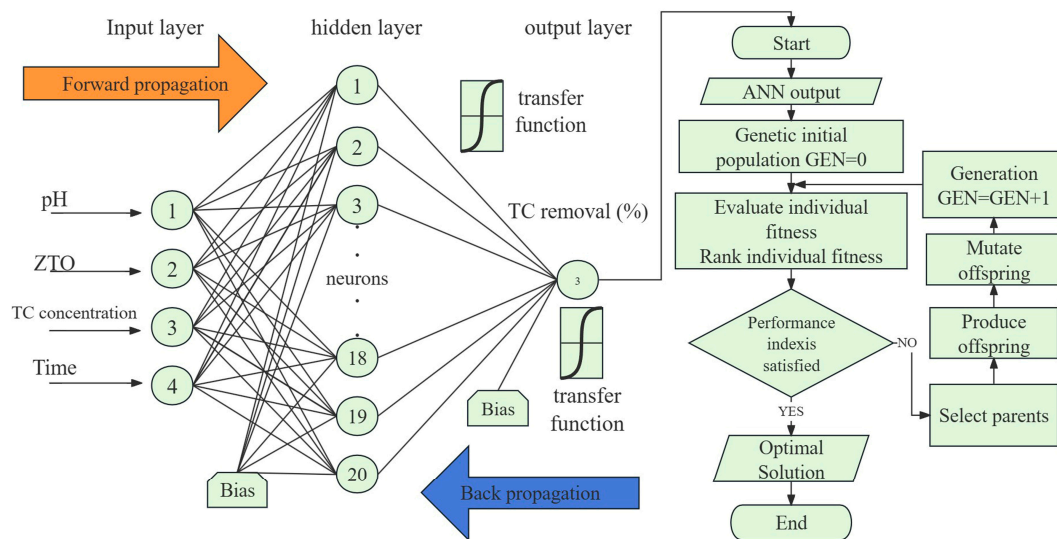


Figure 3. Artificial neural network–genetic algorithm (ANN-GA) model and prediction process [73]. Adapted from ref. [73]. Copyright © 2019 Desalination Publications.

The error between the predicted degradation percentage of TC by the artificial neural network model optimized by a genetic algorithm and the experimental value is only 1.02%. Gradually, artificial neural network models optimized by genetic algorithms are widely used to predict the photocatalytic performance of photocatalysts [75–77].

4.2. Neural Network Model Optimized by Whale Algorithm

The whale algorithm is a kind of intelligent optimization algorithm that solves optimization problems by simulating the behavior of whales [78]. The whale's main actions during iteration include surrounding prey, capturing prey, and searching for prey [79]. When hunting, whales surround their prey and update their position by surrounding their prey, as follows:

$$\vec{D} = \left| \vec{C} \times \vec{X}^*(t) - \vec{X}(t) \right| \quad (15)$$

$$\vec{X}^*(t+1) = \vec{X}^*(t) - \vec{A} * \vec{D} \quad (16)$$

where D and t represent the number of variables solved in the problem and the current number of iterations, respectively. $\vec{A}$ and $\vec{C}$ represent the coefficient. $\vec{X}^*(t)$ and $\vec{X}(t)$ represent the position of the whale with the best fitness at present and the position of the whale in the current number of iterations, respectively. A and C are obtained from Equations (17) and (18), respectively.

$$\vec{A} = 2\vec{a} \times \vec{r} - \vec{a} \quad (17)$$

$$\vec{C} = 2 \times \vec{r} \quad (18)$$

Here, $\vec{r}$ is a random number in the range (0, 1), and the $\vec{a}$ value decreases from 2 to 0. The purpose of hunting prey is to find a better solution.

$$\vec{D} = \left| \vec{C} \times X_{\text{Rand}} - \vec{X} \right| \quad (19)$$

$$\vec{X}(t+1) = X_{\text{Rand}} - \vec{A} \times \vec{D} \quad (20)$$

Here, X_{Rand} is a random whale position. When whales hunt, they swim toward their prey in a spiral motion, as follows:

$$\vec{X}(t+1) = \begin{cases} \vec{X}^*(t) - \vec{A} \times \vec{D}, & p < 0.5 \\ \vec{X}^*(t) - (\vec{X}^*(t) - \vec{X}(t)) \times e^{bl} \times \cos(2\pi l), & p \geq 0.5 \end{cases} \quad (21)$$

where p is the probability, taking the value 0 to 1, b is a constant, representing the shape of the spiral, and l is a random number, in the range $(-1, 1)$. The whale algorithm model is customized to accurately predict the photocatalytic performance of the photocatalyst when the artificial neural network model is employed to train the experimental data. However, the application of the whale algorithm optimized neural network model to the prediction of the photocatalytic performance of photocatalysts is still immature, and only a small amount of work has been carried out to predict the photocatalytic performance [80]. Based on our earlier work, the neural network model optimized by the whale algorithm for predicting the photocatalytic activity of $\text{MgAl}_2\text{O}_4/\text{C}_3\text{N}_4/\text{YMnO}_3$ photocatalysts is shown in Figure 4. In this model, the mass percentage of each component and irradiation time are taken as input parameters, and the absorbance curve value at 255–438 nm wavelength is taken as output parameters to train the neural network model [81]. The model is optimized by combining the whale algorithm after training the neural network model, which improves its ability to predict the photocatalytic performance of the $\text{MgAl}_2\text{O}_4/\text{C}_3\text{N}_4/\text{YMnO}_3$ photocatalyst.

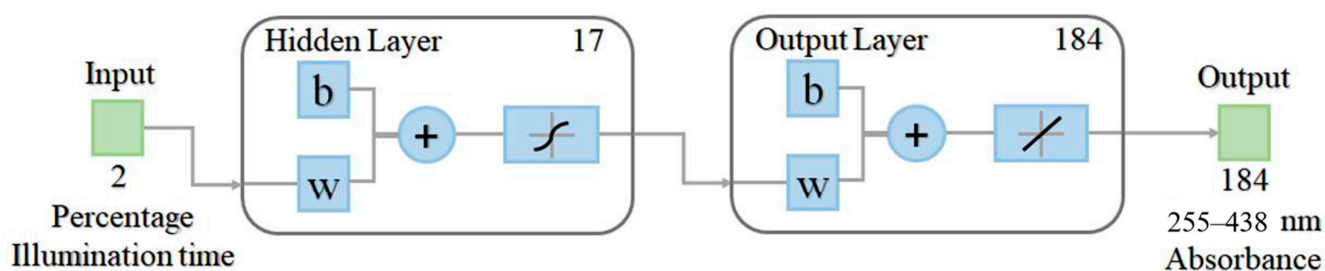


Figure 4. Neural network model optimized by whale algorithm to predict photocatalytic activity of $\text{MgAl}_2\text{O}_4/\text{C}_3\text{N}_4/\text{YMnO}_3$ photocatalysts [81]. Adapted from ref. [81]. Copyright © 2022 The American Ceramic Society.

4.3. Neural Network Model Optimized by Sparrow Search Algorithm

Inspired by the foraging behavior and anti-predation behaviors of sparrows, a new intelligent optimization algorithm, known as the sparrow search algorithm, was proposed in 2020 [82]. In the process of foraging, the sparrows are divided into two categories including explorers and followers [83]. The explorer is responsible for finding food in the population and providing foraging areas and directions for the entire sparrow population,

while the followers use the explorer to obtain food [84,85]. The position of the sparrow when it finds food can be described by the following matrix [82]:

$$X = \begin{bmatrix} x_{1,1} x_{1,2} \dots x_{1,d} \\ x_{2,1} x_{2,2} \dots x_{2,d} \\ \dots \dots \dots \dots \\ x_{n,1} x_{n,2} \dots x_{n,d} \end{bmatrix} \quad (22)$$

The following expression can be used to describe the fitness value of the sparrows:

$$F_x = \begin{bmatrix} f([x_{1,1} x_{1,2} \dots x_{1,d}]) \\ f([x_{2,1} x_{2,2} \dots x_{2,d}]) \\ \dots \dots \dots \dots \\ f([x_{n,1} x_{n,2} \dots x_{n,d}]) \end{bmatrix} \quad (23)$$

The explorer's position update can be expressed in the following way during each iteration [86]:

$$X_{i,j}^{t+1} = \begin{cases} X_{i,j}^t \times \exp(\frac{-i}{\alpha \times \text{iter}_{\max}}), & R_2 < ST \\ X_{i,j}^t + Q \times L, & R_2 \geq ST \end{cases} \quad (24)$$

where $\alpha \in [0, 1]$, $R_2 \in [0, 1]$ and $ST \in [0.5, 1.0]$. Q is a normally distributed random number. L is $1 \times d$ dimension matrix.

With each iteration, the position update of the follower can be expressed as follows [82]:

$$X_{i,j}^{t+1} = \begin{cases} Q \times \exp(\frac{X_{\text{Worst}}^t - X_{i,j}^t}{i^2}), & i < \frac{n}{2} \\ X_p^{t+1} + |X_{i,j}^t - X_p^{t+1}| \times (A^T (A A^T)^{-1}) \times L, & \text{Otherwise} \end{cases} \quad (25)$$

where X_p and X_{worst} are the optimal position and the worst position, respectively.

When aware of danger during predation, the sparrow population will engage in anti-predation behavior, which can be described as follows [82,87,88]:

$$X_{i,j}^{t+1} = \begin{cases} X_{\text{Best}}^t + \beta \times |X_{i,j}^t - X_{\text{Best}}^t|, & f_i > f_g \\ X_{i,j}^t + K \times (\frac{|X_{i,j}^t - X_{\text{Worst}}^t|}{(f_i - f_w) + \epsilon}), & f_i = f_g \end{cases} \quad (26)$$

where X_{Best} and β are the current global optimal position and the control parameter, respectively. $K \in [-1, 1]$. f_i , f_g , f_w , and ϵ are the fitness values of the present sparrow, the current global best value, the current worst fitness value, and the smallest constant, respectively. Yang et al. [89] established an artificial neural network model optimized by the Sparrow search algorithm to predict the photocatalytic performance of $\text{BiVO}_4/\text{BiPO}_4/\text{rGO}$ heterojunctions. The calculation flow chart and model diagram are depicted in Figure 5. The input parameters were the pH value of the reaction solution, the content of BiVO_4 , the content of GO, and the volume of ethanol. The output parameter is the degradation rate of methylene blue. The number of hidden layer nodes can be adjusted between 2 and 15. To achieve an optimized neural network, it is important to aim for the most effective number of hidden layer nodes. The training set accounts for 75% of the total data, while the test and validation sets account for 15%. The degradation percentage predicted by the neural network model optimized by the sparrow search algorithm is 98.2%, and the error with the experimental value is only 0.9%. The optimized values of pH, content of BiVO_4 , GO content, and ethanol volume were 10, 0.14 mg, 33.5 mg, and 19.9 mL, respectively. The sparrow search algorithm has been shown to accurately predict the photocatalytic performance of multi-heterojunction photocatalysts, as evidenced by the results.

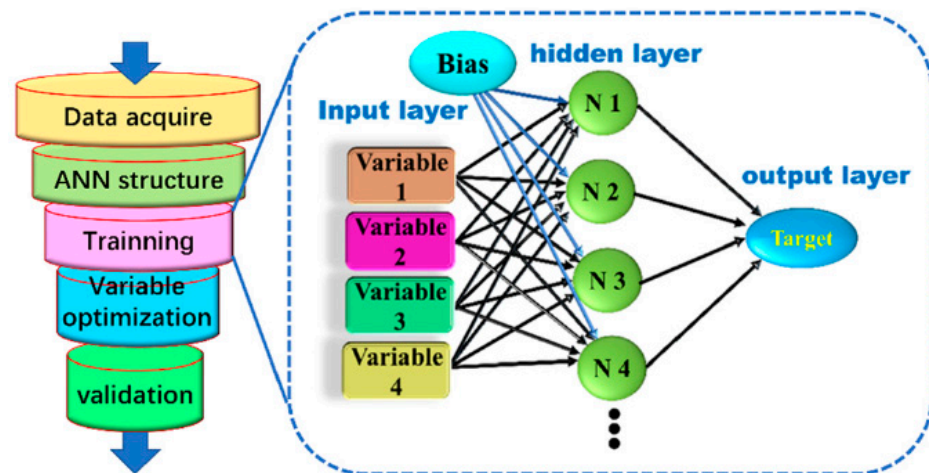


Figure 5. Neural network model optimized by sparrow search algorithm of BiVO₄/BiPO₄/rGO heterojunctions [89]. Adapted from ref. [89]. Copyright © 2023 Elsevier B.V.

4.4. Neural Network Model Optimized by Particle Swarm Algorithm

The particle swarm optimization (PSO) algorithm is an evolutionary computing technique that was invented by J. Kennedy and R. C. Eberhar in 1995 and was created by simulating a popular social model [90,91]. Assuming a particle swarm exists in an m-dimensional space, the position of particles can be expressed by Formula (27) [92].

$$\Psi_j = [\Psi_{j1}, \Psi_{j2}, \dots, \Psi_{jm}]^T \quad (27)$$

The velocity of the particles can be expressed by the Equation (28).

$$v_j = [v_{j1}, v_{j2}, \dots, v_{jm}]^T \quad (28)$$

The optimal position of an individual particle can be described by Equation (29).

$$\varphi_j = [\varphi_{j1}, \varphi_{j2}, \dots, \varphi_{jm}]^T \quad (29)$$

Additionally, the optimal position for the entire group can be described using Equation (30).

$$\theta_j = [\theta_{j1}, \theta_{j2}, \dots, \theta_{jm}]^T \quad (30)$$

The particle's position and velocity are updated after each iteration and can be described by Equation (31).

$$\begin{cases} v_{jd}^{t+1} = \tau v_{jd}^t + l_1 R_1 (\varphi_{jd}^t - \Psi_{jd}^t) + l_2 R_2 (\varphi_{jd}^t - \Psi_{jd}^t) \\ \Psi_{jd}^{t+1} = \Psi_{jd}^t + v_{jd}^{t+1} \\ d = 1, 2, \dots, t \end{cases} \quad (31)$$

Here, l and R are numbers between 0 and 1. Owolabi et al. [92] used a support vector regression model optimized by a particle swarm optimization algorithm to predict the band gap values of bismuth oxychloride wide-bandgap semiconductors. The influence of lattice oxygen and oxygen vacancy on the band value of bismuth oxychloride semiconductors is discussed by the trained model. Karri et al. [93] predicted the (II) removal efficiency of activated carbon based on palm kernel shell by using a neural network model optimized by particle swarm optimization algorithm. Figure 6 shows the neural network model optimized by the particle swarm optimization algorithm (ANN-PSO) model. With the initial concentration, pH, activated carbon dosage, residence time, and reaction temperature as input parameters and Zn(II) removal efficiency as output parameters, the effects of these

environmental parameters on Zn(II) removal efficiency were discussed. The R^2 value is above 0.91, indicating that the model can effectively predict the removal efficiency of Zn(II) from palm kernel shell-based activated carbon.

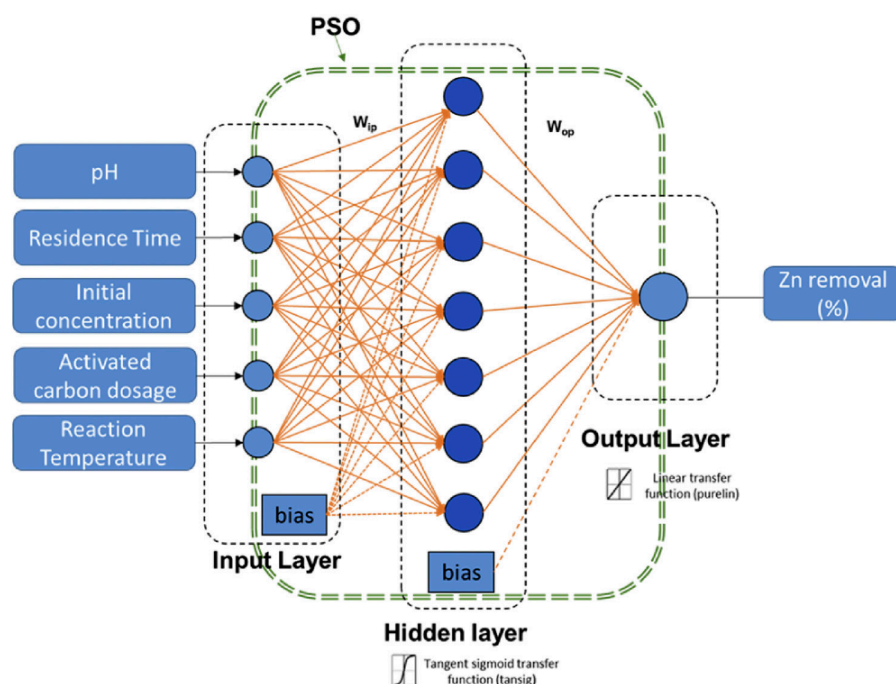


Figure 6. Neural network model optimized using particle swarm optimization algorithm (ANN-PSO) model [93]. Adapted from ref. [93]. Copyright © 2017 Elsevier Ltd.

5. Practical Application in the Field of Photocatalysis

The rapid advancement of artificial intelligence has led to its unprecedented application in the field of photocatalysis. The application of intelligent algorithms in the field of photocatalysis mainly includes three aspects. (1) The photocatalytic activity of the photocatalyst is closely related to the energy band (E_g) value of the semiconductor material, and the intelligent algorithm is closely combined with the first-principles calculation to develop the new photocatalyst efficiently and quickly. (2) The degradation rate of the photocatalyst was predicted using intelligent algorithms after exploring the influence of various environmental parameters on its photocatalytic activity. (3) There is a dependence between the degradation rate and absorbance of photocatalysts. The absorbance curve of the reaction solution under different environmental parameters is trained by an intelligent algorithm to predict the photocatalytic activity of photocatalysts.

5.1. Intelligent Algorithm Combined with DFT Calculation to Develop New Photocatalyst

The application of intelligent algorithms in the field of photocatalysis largely depends on the characteristics of the model, as well as the structure and type of data [94]. The obtained experimental data or theoretical calculations can only be calculated and predicted if they are suitable for building a matrix that conforms to the neural network model. According to the following Formula (32), it is possible to determine if the material is a semiconductor.

$$E_g(\text{eV}) = \frac{1240}{\lambda(\text{nm})}, 0.5 < E_g < 3.5 \quad (32)$$

By predicting the E_g value of a semiconductor material, it is possible to determine whether the semiconductor material can potentially be used in the field of photocatalysis. Wan et al. [95] collected a series of data such as molecular components, space groups, experimental E_g values, and E_g values obtained from density functional theory (DFT) calculations of semiconductor materials, and then built a neural network model to predict

the E_g values of these semiconductor materials. The corresponding model can be described as follows:

$$E_g(\text{ANN}) = W_2[\text{ReLU}(W_1X + b_1) + b_2] \quad (33)$$

$$\text{ReLU}(x) = \max(0, x) \quad (34)$$

where W_1 and W_2 are the weight matrices. b_1 and b_2 are the bias vectors. In addition, with the following parameters as input parameters—the PBE functional (E_g (PBE)), the total number of electrons (N_e), the average number of electrons in each atom ($N_e\%$), the total number of atoms (N), the space group (G), the number of constituent elements (E_N), and the number of transition atoms (N_T) [91]—the model can be improved as follows:

$$X = \begin{bmatrix} E_g(\text{PBE}) \\ N_e\% \\ N \\ G \\ E_N \\ N_T \end{bmatrix}^T \quad (35)$$

The improved artificial neural network model is capable of accurately predicting the E_g values of various solid materials, which can reduce the cost of computing resources. Meanwhile, the element composition, atomic radius, atomic mass, the volume of each atom, grain size, and cell parameters also have a great influence on the E_g value of semiconductor materials [96–100]. Na et al. [101] proposed using the tuplewise graph neural network (TGNN) algorithm model to predict the E_g values of 45,835 semiconductor materials mainly based on some public database data obtained by DFT calculation. Figure 7 shows the TGNN model for predicting the E_g values of 45,835 semiconductor materials. Five processes are primarily involved in the model: crystal structure transformation, determination of output nodes and boundary conditions, graph insertion, crystal-level property transformation, and target property prediction [101]. The model is capable of predicting the E_g values of other materials with higher accuracy than the standard density functional theory calculation. In short, the structure–function relationship between the crystal structure information of semiconductor materials and its E_g value is established, and the intrinsic relationship between the E_g value and the photocatalytic activity of semiconductor materials is established, so as to achieve the prediction of the photocatalytic activity of new photocatalysts.

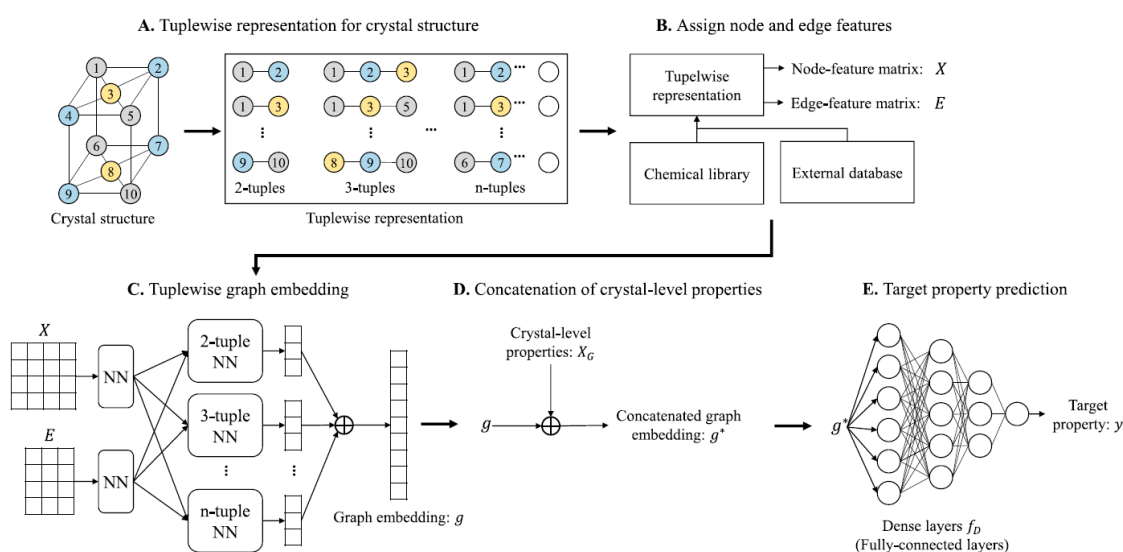


Figure 7. Tuplewise graph neural network (TGNN) model [101]. Here, $g^* = g \oplus X_G$, X_G is the input of crystal-level properties. Adapted from ref. [101]. Copyright © 2020 American Chemical Society.

5.2. The Intelligent Algorithm Optimally Calculates the Degradation Percentage of Photocatalyst

There are many parameters that affect the photocatalytic performance of photocatalysts, including catalyst content, initial concentration of pollutants, pH value, irradiation time, catalyst particle size, optical band gap value, etc. [102–108]. The effect of various parameters on the photocatalytic performance can be designed by the response surface method, and then the law of the effect of each parameter on the photocatalytic performance of the photocatalyst can be studied. The degradation percentage (DP%) of pollutants degraded by semiconductor materials can be approximated by the following Formula (38):

$$DP\% = (1 - \frac{C_t}{C_0}) \times 100\% \quad (36)$$

where C_0 and C_t are the concentration of pollutants at the initial time and the concentration of pollutants at the time t , respectively. Berkani et al. [109] used a neural network model combined with a response surface method to predict the photocatalytic performance of TiO_2 for the degradation of Basic Red 46 dye. The results show that the degradation percentage obtained by the response surface method is highly consistent with that predicted by the neural network model.

Antonopoulou et al. [110] used the feed-forward multilayered perceptron (MLP) combined with the response surface method to predict the photocatalytic degradation percentage of total phenolic by TiO_2 photocatalyst. The MLP model can be described as follows:

$$v(u) = g_2(\sum_{k=1}^K w_k \times g_1(\sum_{l=1}^L w_{kl} \times u_l + w_0) + w_0) \quad (37)$$

The training function can be expressed by Equation (37):

$$\Delta w(t+1) = -\mu \times \frac{\partial E}{\partial w} + \beta \times \Delta w(t) \quad (38)$$

According to the results, the neural network model is more accurate than the response surface method. The MLP model has also been used to predict the degradation activity of TiO_2 in degrading Bisphenol A [111]. At present, many models, such as the support vector machine, multilayered feed-forward network, generalized additive model, convolutional neural network, adaptive neuro-fuzzy inference system, big data analysis, and deep learning models, have been used to predict the photocatalytic performance of photocatalysts [112–119]. It is worth noting that it is difficult for a single neural network model to meet the demand of prediction, and multiple models combined with training corresponding experimental data can effectively predict the photocatalytic performance of photocatalysts. Jiang et al. [120] employed the crystal graphic convolutional neural network–molecular fingerprint–artificial neural network (CGCNN-MF-ANN) to predict the photocatalytic performance of a variety of different photocatalysts. Figure 8 shows the structure of the CGCNN-MF-ANN model. A new type of semiconductor photocatalyst can be designed using this model.

5.3. The Intelligent Algorithm Optimizes the Absorbance Curve and Then Predicts the Photocatalytic Activity of the Photocatalyst

Within a certain concentration range, the absorbance value is linearly dependent on the concentration value. Hence, the DP% of pollutants degraded by semiconductor materials can be approximated by the following Formula (39):

$$DP\% \approx (1 - \frac{A_t}{A_0}) \times 100\% \quad (39)$$

where A_0 and A_t are the absorbance value of pollutants at the initial time and the concentration of pollutants at the time t , respectively. When the ultraviolet visible spectrophotometer is used to test the pollutants with different irradiation times, the absorbance curves of different times are obtained. It is no longer just one value as measured by the 721 powder

photometer, but a curve. In addition to the above prediction of the degradation percentage of pollutants, the absorbance curve of the degraded pollutants can also be predicted, and the degradation percentage of pollutants can be calculated through Formula (39). The measurement process of photocatalysis can be more dynamically reflected by predicting the absorbance curve. For the prediction of the above degradation percentage, it belongs to the multi-input single-output model. However, the prediction of the absorbance curve belongs to the model of input and output, which is more difficult. Hassanien et al. [121] designed a backpropagation (BP) neural network model based on different experimental parameters such as TiO_2 , H_2SO_4 , NaIO_4 , $\text{K}_2\text{S}_2\text{O}_8$, dye, and silver nitrate. Training and prediction of the maximum peak value of absorbance curves of degraded pollutants were conducted using six different optimization algorithms. This model can be described by Formula (40).

$$Y = f \left[v_0 + \left(\sum_{i=1}^m (\lambda_i + \sum_{j=1}^n x_j w_{ij}) \right) v_j \right] \quad (40)$$

By improving this model, an optimized BP neural network model is established.

$$P_i^l = \sum_{j=1}^n w_{ij}^{(l)} x_j^{l-1} + b_j^{(l)} \quad (41)$$

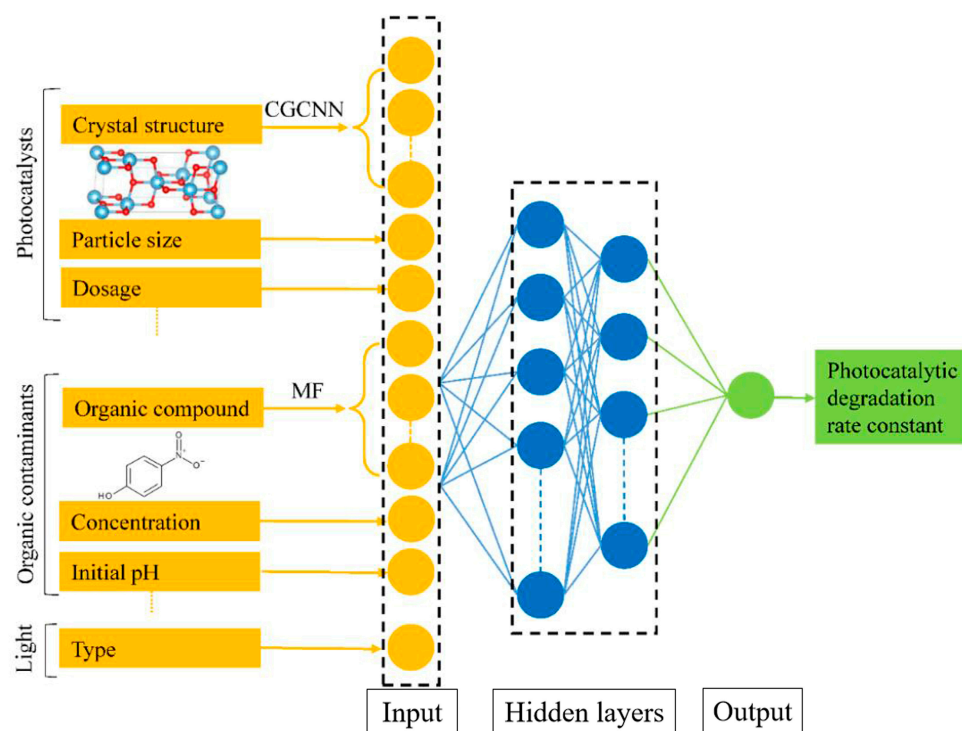


Figure 8. Crystal graphic convolutional neural network–molecular fingerprint–artificial neural network (CGCNN-MF-ANN) model [120]. Adapted from ref. [120]. Copyright © 2021 by the authors.

By comparing different models, it was found that the optimized BP neural network model has the best effect in predicting the absorbance value of Acid Black 24 textile dyes degraded by photocatalyst. Generally, the absorbance value of degraded pollutants is measured using a spectrophotometer, and the absorbance curve is obtained using this device. Therefore, the absorbance curve of degraded pollutants can be predicted directly using different environmental parameters, and the degradation percentage of pollutants can be obtained in an intuitive manner. In our earlier work, the removal ability of $\text{MgAl}_2\text{O}_4/\text{C}_3\text{N}_4/\text{YMnO}_3$ [81] and $\text{CeO}_2/\text{YMnO}_3$ [122] composite photocatalysts for dye removal was predicted by an intelligent algorithm-optimized neural network model. Figure 9 shows the neural network model for the predicted adsorption capacity of $\text{CeO}_2/\text{YMnO}_3$ composite photocatalysts. The model takes the mass percentage of YMnO_3 and CeO_2 and

irradiation time as the input parameters, and the absorbance value of 280–600 nm wavelength as the output parameters for training. Finally, the whole network is trained using a neural network model optimized by the genetic algorithm and the whale algorithm. The results show that the neural network model optimized by genetic algorithms has the best prediction ability. Simultaneously, the neural network model has a certain prediction range when predicting the photocatalytic performance of the photocatalyst, which is influenced by the selected training parameters, prediction accuracy, and reliability. The photocatalytic performance of each value can be reliably predicted within the range of each parameter, but it is difficult to predict accurately beyond this range [122]. Similarly, the emergence of many new photocatalysts and some new parameter variables makes the simulation prediction of neural networks more complicated, which requires the development of some new neural network models to adapt to the rapid development of photocatalysis research [123–125].

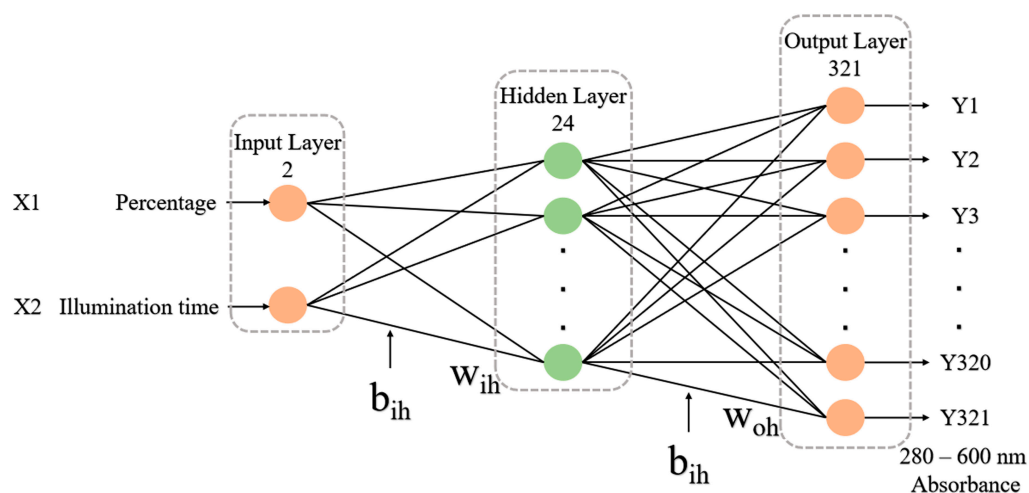


Figure 9. Neural network model for the predicting adsorption capacity of $\text{CeO}_2/\text{YMnO}_3$ composite photocatalysts [122]. Adapted from ref. [122]. Copyright © 2022 Elsevier B.V.

6. Conclusions and Prospect

6.1. Conclusions

In the 21st century, artificial intelligence continues to rise, making it play an irreplaceable role in all walks of life. In particular, the application of machine learning to the design of photocatalysts and the prediction of photocatalytic performance has made research in the field of photocatalysis more promising. This paper reviews the computational process of machine learning algorithms in the field of photocatalysis, and the database, algorithm model, software, parameter setting, training, and prediction used in the calculation process. The neural network model and its improvement based on an intelligent optimization algorithm are discussed in detail. The development of new photocatalysts by combining intelligent algorithms and density functional theory, and the prediction of photocatalytic performance of photocatalysts by combining intelligent algorithms and neural network models are discussed. The purpose of this review is to provide theoretical reference and technical support for the use of intelligent algorithms in the development of new photocatalysts and to predict the photocatalytic performance of photocatalysts.

6.2. Prospect

The application of intelligent algorithms in the field of photocatalysis is still in its infancy, and many new intelligent algorithms need to be explored to make them applicable to photocatalysis research. In future research, the following work can also be carried out:

- (1) The development of many intelligent algorithms is still ongoing. These newly discovered intelligent algorithms can be applied in photocatalysis to expand their use in interdisciplinary fields and promote the development of photocatalysis technology.

In particular, combining and matching the algorithm model with experimental data, theoretical calculation data, and data from other databases to make it suitable for the calculation, training, and prediction of the model can also promote the improvement of the model and trigger the development of new models.

- (2) It is difficult for a single algorithmic model to meet the requirements of calculation, training, and prediction, so it is necessary to combine a variety of algorithmic models to make use of the advantages of these algorithms to better predict the photocatalytic performance of photocatalysts. The integration of multiple models requires relatively difficult technology, which limits the application of intelligent algorithms in the field of photocatalysis to a certain extent.
- (3) Most neural network models have multiple inputs and only one output, but research on multiple input and multiple output models is relatively rare. The application of a neural network model optimized by an intelligent algorithm in the field of photocatalysis is a technical challenge.
- (4) Explore the development of new intelligent algorithms for training and predicting the photocatalytic performance of photocatalysts. The development of intelligent algorithms suitable for the prediction of the photocatalytic performance of different photocatalysts will promote the development of photocatalytic technology, shorten the time required to develop new photocatalysts, and save costs.

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