

RESEARCH PROGRESS OF ARTIFICIAL INTELLIGENCE IN THE FIELD OF RENEWABLE ENERGY MATERIALS RESEARCH AND DEVELOPMENT

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Abstract: In recent years, traditional energy sources such as coal, oil, and natural gas have been gradually depleted, and the use of large amounts of fossil energy has caused environmental pollution. In order to reduce carbon dioxide emissions, the country actively promotes wind, The development of renewable energy sources such as light, hydropower, and hydrogen energy, and the key to the promotion and application of these energy technologies is the research and development of new materials. At present, the development of new materials mainly relies on researchers to conduct experimental optimization based on the material structure and its expected catalytic activity for a specific system, resulting in a slow development process of new materials. With the further development of computational materials science, researchers have integrated a large number of material databases on material structure and performance characterization, and gradually optimized and screened new materials through comparison. This paper reviews the current design ideas and synthesis methods of material development, focusing on artificial intelligence (AI) and expounding the recent research based on AI Method design, models and algorithms in the process of preparing renewable energy materials, and summarized AI The research significance and development process used in material design, and finally the AI Methods The development of design and preparation of renewable energy materials is prospected, the material optimization model proposed by this research group is introduced, and cases of the model's successful application in material optimization for hydrogen evolution from electrolysis of water and hydrogen production from sodium borohydride are listed. The future, AI The technology has very broad application prospects in theoretical calculations, synthetic design, performance prediction, and material microstructure characterization analysis of new materials.

Keywords: Material preparation; Artificial Intelligence (AI); Renewable energy; Material optimization

1 MATERIAL DESIGN METHODS

Looking at the situation at home and abroad, traditional energy sources such as coal and oil are gradually depleted, resulting in endless environmental problems. Among them, greenhouses The massive emission of gaseous carbon dioxide has caused serious pollution to the atmosphere. dye. No. The 75th United Nations General Assembly proposed that China reach carbon emissions targets by 2030 Peak, 2060 Carbon neutrality target task before the year [1]. To realize this country Strategic goals, the country actively supports the development of renewable energy, such as Wind, light, electricity, hydro energy, and the promotion and application of new energy technologies are inseparable from Open up efficient research and development of new materials.

At present, the research and development of new materials mainly relies on the practical operation and scientific intuition of R&D personnel, and the material objects are very complex, which need to be determined according to their own structure and their expected catalytic activity for a specific system. Experimental optimization of properties, etc., which leads to new materials from material development to The market cycle is very long [2]. With the development of science and technology, through long-term research by various scientific researchers, methods of material development have gradually taken shape. A relatively mature material development method. For example, template technology [3] When used in the preparation of nanomaterials, the morphology, structure, size and other characteristics of nanomaterials can be controlled. Chemical methods were used to obtain trace etched polymer templates (TEPM) [4], mesoporous molecules were used to screen out mesoporous materials [5], and carbon nanotube structures were used to obtain carbon nanowires [6] etc., which can not only increase the output of nanomaterials, but also solve some stability problems encountered in the synthesis of nanomaterials. In the preparation of inorganic nanomaterials, microemulsification technology [7] can overcome the limitations of traditional methods, adopt various forms with larger strength, size and solubilization amount, and produce various chemical effects on inorganic nanomaterials. reaction. However, in the process of preparing inorganic nanomaterials using microemulsification technology, since the prepared emulsion has a great impact on the structure and material exchange rate of inorganic nanomaterials, multiple experiments are required to optimize the preparation of inorganic nanomaterials with optimal structure and material exchange rate. nanomaterials.

In recent years, artificial intelligence (AI) technology has become increasingly mature. Workers in fields such as diagnostics, medical engineering, petroleum industry and aerospace Significant progress has been made in the application of engineering [8]. Further developments in computational materials science The development has formed a large number of material databases, deep learning (Deep Learning, DL), density functional theory (DFT) and high-

throughput calculations, etc. Mature theories provide computational theoretical models. Based on this, use AI optimizes material composition and process parameters, combined with material stability and selection Selectivity and catalytic activity in specific fields are used to screen new materials. This method has changed the research and development model of new materials and improved the efficiency of materials research and development. Improve efficiency and accelerate the research and development process of new materials.

1.1 Material Index Method

The material index method [9] is used to determine the quality of various structural materials. Quantity estimation, each new material can be calculated by calculating its index numbers and compared characterization with the indices of currently used materials. this This method was introduced by Gustav in 1960 Niemann Founded, mainly through By describing some quantitative properties of each material and how the material is used Quantitative assessment in use, using simple functional forms to calculate materials The amount of material used. This method is simpler and more convenient to implement, and it can also Use the descriptive classification criteria you selected earlier to select the materials you need Materials can be coded qualitatively or quantitatively.

1.2 Nanotopology Optimization Method

Nanotopology optimization method [10] controls the size and elasticity of atoms. Design nanoscale materials in terms of properties and other aspects, and find the optimal shape and material distribution of atoms to optimize the performance of the material. Figure 1 exhibition Discovered nanotechnology to design through atomic control at the nanometer scale Materials method steps, where, V^* To define the target volume fraction, r_{min} is the filter radius, α_r is the rejection rate, α_a is the admission rate ($\alpha_r > \alpha_a$). Two different line types of arrows represent two optimization stages. This kind of The method allows the computer to directly design the original material of the required material. sub, thus simplifying the complexity of material design.

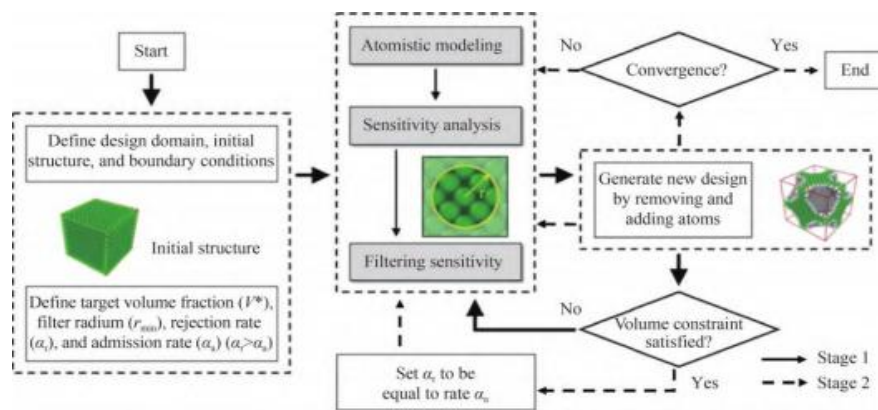


Fig. 1 Methods for designing materials through atomic control at the nanoscale

1.3 Topology Optimization Method Based on Deformation Energy

The design of highly ductile materials faces the challenge of preparing materials The problem of gradual failure is the problem of gradual failure, so the main goal of the topology optimization method based on deformation energy [11] is to minimize the unit distortion energy and ensure that the deformation under a certain load does not exceed the unit failure limit. The most effective way is to use p- norm This function will The data points of a substance are all gathered into an objective function (formula (1, 2) [11], under the constraints of the material volume, the torsion function can be used to The value of the curve energy is minimized as much as possible, where MN yes p The norm function minimizes the distortion energy, p is the norm factor, $E_i(x)$ is the distortion energy of each element, $V(x)$ is the volume of the design, $|\Omega|$ is the total volume of the initial fixed design domain, v_i is the prescribed volume constraint, N is the element number.

$$\min M_{Mon} = \left[\frac{1}{N} \sum_{i=1}^N (E_i(x))^p \right]^{\frac{1}{p}} \quad (0 < x < 1) \quad (1)$$

$$\text{subject to } \frac{V(x)}{|\Omega|} - v_i \leq 0 \quad (2)$$

1.4 Materials Genome Approach

The main research direction of the materials genome method [12] is to study materials R&D conducts “high-throughput” research. Through high-throughput computing, Qualcomm quantitative preparation and characterization, systematic screening and optimization of materials, from And get a new material with excellent properties. for different Materials have different calculation methods for their ion transport properties, Table 1 right 3 A brief

overview of ion transport properties is given. For needs In situations where high-throughput screening of materials is required on a large scale, chemical The learned bonding method can quickly simulate the ion transport path and Migration barrier to achieve rapid and effective screening. For research orders needed In the case of ions, it is necessary to use the DFT The transition state calculation formula of Only by using this method can we accurately analyze the paths and potential barriers of ion transport, but This research method cannot achieve rapid research on ions.

Table 1 Methods for calculating ion transport properties and corresponding calculation amounts

Parameters	Geometry structure	Chemical bonding	Energy change
Principle	Li + moves in a certain geometric space in lattice	Li+ moves in lattice where bond valence mismatch is small	Li+ moves on a migration path with a low energy barrier
Methods	Voronl-Dirichlet Colony Procrystal	Bond valence and theory Valence-based force field method	DFT + transition state theory Molecular dynamics Monte Carlo Simulation

1.5 Uniform Design Method

The uniform design method [13] is a method where the test points are evenly distributed within the test range. Evenly distributed experimental design method, compared with single variable experiment and multi-variable experiment Variable experiments are more representative. Univariate tests because each component Interaction does not yield the best results, and multivariate experiments require more When the quantity is large, the workload will become particularly heavy, and the uniform design method Since the test points are evenly distributed, there is no need to consider the relationship between each component. interaction, while using computers to process experimental data The processing results can be analyzed quickly and accurately.

2 AI AND ITS APPLICATION IN TRADITIONAL MATERIALS

2.1 AI Brief Description

AI is a field of research and development used to simulate, extend and expand human The technical science of intelligent theories, methods, technologies and application systems learning, the basic principle is: the computer will pass the sensor (or artificial input method) to collect real-life information about a situation, and then The information collected is compared with the information stored in the computer Compare, use the compared results to determine the meaning of the collected information, and calculate various possible scenarios based on this information. possibility and predict optimal performance [14]. Artificial Intelligence Algorithm Main point for two big kind,one kind yes base At system count of machine device study Xi(machine learning, ML) algorithm, the other is D.L. algorithm. As shown in the Figure 2 As shown, Lee [15] introduced the relationship between them using representative algorithms. relationships and characteristics of each algorithm. ML According to the learning method, the algorithm can It can be divided into supervised learning, semi-supervised learning, unsupervised machine learning and reinforcement learning [15]. Supervised learning is often used in classification and regression problems With semi-supervised learning, use these two algorithms for these problems It will have better results; unsupervised learning is mostly used for association rules and clustering problems, and performs outstandingly on these problems; reinforcement learning is often used when dealing with problems that interact with the environment. D.L. The algorithms mainly include convolutional neural network (CNN) and recurrent neural network. (RNN), Generative Adversarial Network (GAN) and fully connected network structure (FC). For this 4 kind of network, table 2 applied to it Compare the range, advantages and disadvantages.

Artificial intelligence	Machine learning			Deep learning
Fuzzy systems	Supervised learning	Unsupervised learning	Evolutionary learning	Deterministic
Expert systems	Classification	Clustering	Genetic algorithms	Deep neural network
	Support vector machine	Hierarchical clustering	Particle swarm optimization	Recurrent neural network
	K-Nearest neighbors	DBSCAN	Swarm intelligence (Ant algorithms)	Convolutional neural network
	Ensemble learning boosting/bagging/ random forests	K-means		Autoencoder
	Logistic regression	K-medoids		Deep Q-learning
		Topic modeling (for text data)	Reinforcement learning	
	Decision trees		Q-learning	Probabilistic
	Naive bayes		Markov decision process	Boltzmann machine
	Neural network		Monte carlo method	Restricted boltzmann machine
	Regression	Dimension reduction	Temporal difference learning	Deep blotzmann machine
	Linear regression	Principal component analysis		Deep belief network
		Latent dirichlet analysis		
	Natural language processing (latent dirichlet allocation,word2vec, t-SNE)			
	Image and speech recognition			

Fig. 2 AI Classification of algorithms [15]

Table 2 Comparison of network structures [16]

Name	Scope of application	Advantages	Disadvantages
CNN	Applicable in most fields, excellent in large image processing applications	Strong model generalization ability Does not require high translation invariance of input data	Prone to gradient dissipation Poor spatial relationship recognition Decreased recognition ability after a large rotation of object
RNN	Suitable for processing sequence data such as audio, language, etc.	Can model sequence content, such as speech, video, etc	Too many parameters Prone to gradient dissipation and gradient explosion problems No feature learning ability
GAN	Suitable for scenarios where samples need to be generated, such as image modeling, etc.	Able to produce better samples Any kind of generator network can be trained Avoid complex Markov processes	Poor model convergence Crashes during training Model is too free and uncontrollable
FC	Suitable for scenarios with simple features, such as housing price prediction, advertisement recommendation, etc.	When there is a large difference between the training set and the test set data, it can ensure that the larger model has a good transfer ability	Too many parameters and slow training Image gets bigger and the number of colors increases Inconvenient to handle high-dimensional data

2.2 AI Applications in Traditional Materials

Steel materials have lower cost and better performance, and are widely used in industry. However, the microstructure of steel is affected by various Parameter influence, that is, different parameters, the microstructure of steel will be different. The same composition will show different shapes. According to steel Researchers at the University of Saarland in Germany have discovered the complex microstructure of materials. use D.L. Convolutional neural network and maximum voting mechanism in the algorithm have great impact on steel Cut and analyze the microscopic image of the material, so as to quickly use the computer to Quickly learn the internal standard microscopic morphology of steel and interact with complex microscopic Compare structural steel materials to quickly and accurately classify steel materials [17].

As shown in the Figure 3 As shown, the ceramic manufacturing industry uses artificial intelligence technology Replace traditional manual work with programmable control devices (PLC) Controlling a variety of production lines and management systems greatly increases the output of ceramic material preparation and reduces raw material and labor costs [18]. use The automatic joint control system can not only effectively and accurately spray dry materials Ensure the continuity and stability of the process, and also ensure the quality of the powder quantity and improve the production efficiency of materials. Adopting ceramic intelligent manufacturing full-process information management and control integration technology, relying on intelligent status tracking Obtaining more comprehensive data can provide multi-functional conditions such as online detection, abnormal alarm and maintenance, and gradually improve the sustainable development strategy of ceramic material preparation.

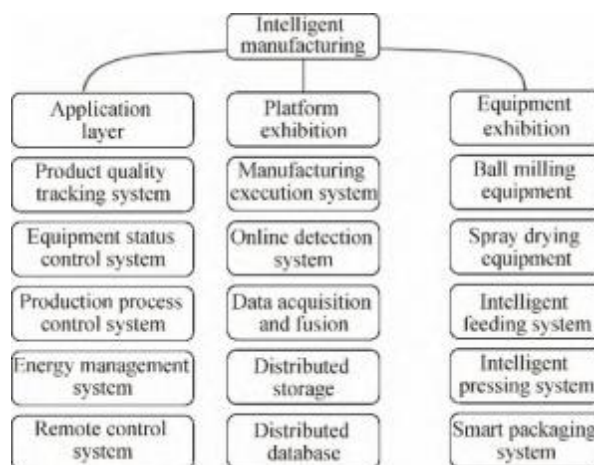


Fig. 3 Overall planning of intelligent manufacturing of ceramic materials

Composite materials are composite products of multiple single metal materials. There are advantages of a single metal material [19], but the design of the material and optimization are also more complex and difficult. Introducing artificial intelligence algorithms into In the research of composite materials, it can effectively accelerate the design and development of materials. Iterate. As shown in the Figure 4 As shown, this process is mainly divided into 3 steps: count Data preparation, model training, and model evaluation. Its applications are mainly divided into Category 3 :

The first is to predict the performance of materials, and the second is to optimize materials performance, and the third is an intelligent optimization of composite materials. Data preparation: For incomplete original data information and redundant data For some other issues, artificial intelligence algorithms can filter data Select and perform preprocessing to increase the efficiency of operations and improve the accuracy of data. accuracy; model training: through supervised learning or unsupervised Learn to predict, identify and judge the properties of materials, so as to Understand the changes in the performance structure of different materials and accurately grasp the differences Computational model of the same material; model evaluation: using algorithms to obtain Compare the results with the test data to identify the model Accuracy of predicted results.

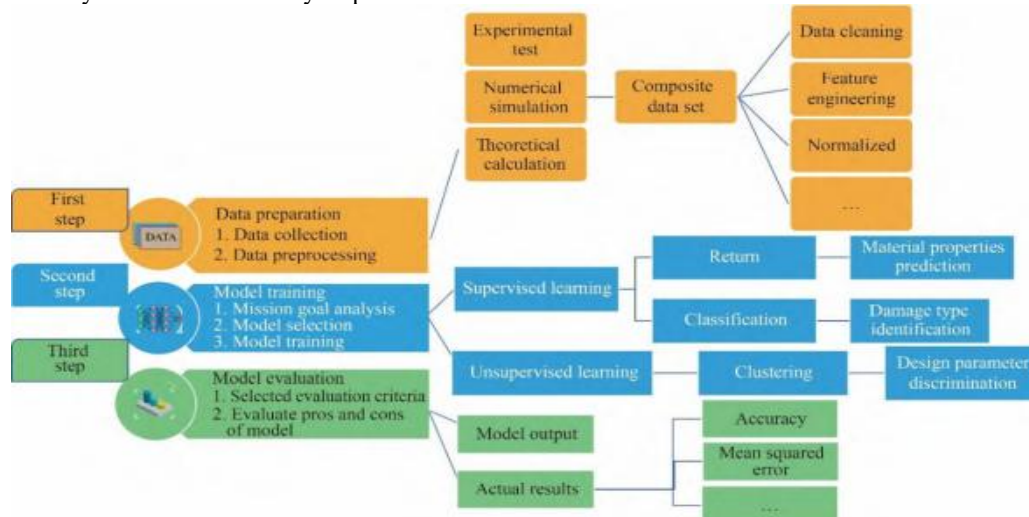


Fig. 4 steps for applying artificial intelligence in composite materials research

3 AI RESEARCH IN RENEWABLE ENERGY MATERIALS PROGRESS

The world is currently facing severe environmental and energy challenges, and coal The continuous consumption of traditional energy sources such as carbon and petroleum has seriously affected humankind's daily life and normal development of society. In order to satisfy the increasing To meet the long-term energy demand, researchers have developed many clean energy technologies, Including new energy technologies such as solar energy, wind energy, electrochemical energy and hydrogen energy technique. To achieve this change, advanced materials must be created to support Support emerging energy technologies. Therefore, the development of more efficient and environmentally friendly energy sources are attracting more and more attention. Renewable energy materials are mainly used for electrochemical energy storage or conversion. For portable electronic products, electrical transportation, integration of intermittent renewable energy into the grid, and many Many other energy or power applications become critical. And energy materials The study of materials depends on multiple variables and parameters, and manual optimization can only It is performed by changing one factor at a time, and there are too many types of research subjects, and the research objects are complex and difficult to control. In order to effectively improve the material design Taking into account the efficiency of research and development, this introduces AI technology.

3.1 Wind Power Materials

Wind energy, as a clean and renewable energy, plays an important role in reducing temperature greenhouse gas emissions and leading the development of sustainable energy systems. occupies a major position and is a promising alternative to traditional fossil fuels Substitutes [20-21]. Zhang et al. [22] proposed that AI and data analysis are applied to wind power systems to improve the performance of wind power and achieve big rules Model wind force Generate electricity. Hong and Rioflorido [23], Lin and Liu [24] proved that artificial neural network (ANN) can better predict wind energy. Wind turbines are key components of wind energy conversion systems Materials that support the capture of kinetic energy from wind energy and convert it into mechanical Mechanical energy [25]. To meet the growing demand for renewable energy, The need continues to develop and install larger, more powerful, longer turbine blades wind turbine. Furthermore, in order to compete with low-cost fossil fuel energy To compete with other sources, wind energy also needs to be delivered at a low level cost of energy (LCOE) Production. The mechanical energy generated due to the rotation of the blades is transmitted to the rotor of the generator, ultimately producing electrical energy. Therefore, the materials of blades and generators Materials are a key element of wind turbines. Pasquali Wait [26] to find smallest LCOE As the goal of component design life, a basic Based on the method of defining component upgrade time based on the optimal life of components, an algorithm optimization problem is designed to find the minimum LCOE component design life. Three parameters are considered : marginal cost of design life cost, the opportunity cost of technological development, and the cost adjustment of time, A constraint creation algorithm based on the interaction between system components is proposed. method, using the evolutionary

optimization method to solve the optimal life of the component, and finally Conduct a sensitivity analysis to determine the most influential design parameters.

Wind power generation system consists of control system, condition monitoring system and Supervisory control and data acquisition (SCADA) system composition. Among them, L in and Liu [24] found that through The SCADA system combines with the wind turbine controller to monitor the overall operating status of the wind farm, which can realize the control of the wind farm. Efficient management. Li [27] and Barbounis et al [28] used RNN separately measure wind energy and wind speed. In an operating wind farm, upstream wind turbines both generate electricity and cause wakes that cause damage to downstream wind turbines. Performance degrades.

In the face of natural disasters such as hurricanes, wood materials such as poles Deteriorating over time, the failure rate of the wind power grid system is extremely easy improve. Qin and Wei [29] used physics-based easy Damage analysis, combining the physical characteristics of pole and wire components and the pole and wire system The topological structure generates the fragile surface of the member. Uncertainties at the material level are propagated to the component level through reliability analysis and finally through Failure rate estimates are propagated to the system level through a Bayesian network (BN) obtains the wind power grid failure rate at each time step (k). use view Measurement arrive of rod pieces lose effect number according to,base At hour between step long of between separated (Δt), the material characteristics of components in wind power systems are analyzed through Bayesian reasoning. Sexuality and vulnerability are updated. This can effectively reduce the cost of wind power systems and promote risk assessment of system degradation.

3.2 Optoelectronic Materials

The development of the world economy essentially depends on efficient methods of generating electricity, format, appropriate management and distribution [30]. Traditional energy generation methods has created huge environmental problems around the world, and its actions are unacceptable Renewable energy sources are gradually depleting, forcing countries to switch from non-renewable The power generation model has shifted to the use of non-polluting and cheaper renewable energy sources such as solar energy, wind energy and tidal energy [31]. sun The solar radiation required to generate electricity is available all year round, and the operation and maintenance costs are low. A better way to generate electricity than wind and tidal energy. And solar energy as Alternative energy sources whose performance improvements are needed to achieve the world's future energy needs An inevitable choice [32].

For the screening of solar cell materials, the key influence The impact factor is Shockley - Quisser limits and band gaps. metal halide Perovskite material is a compound with adjustable formula and easy preparation. made, and has advantages such as high carrier lifetime and adjustable absorption band gap. Human optoelectronic performance, power conversion efficiency (PCE) in just ten years reached from 3.8% to 25.5% change [33]. Although perovskite type solar cell (PSC) with high PCE and excellent material properties, but the best performance PSC Poor long-term environmental stability still exists problem [34-36]. Research has found that PSC Industrial applications are still improving space, adjusting the perovskite composition or using additives [37] can change improve the phase change efficiency and stability of the device, so many researchers propose ML model type All concentrated exist calcium titanium mine material material on [38]. Allam Wait [39] to use DFT Computational and neural network models analyze metal halides compound perovskite band gap and determined for training ML model The Importance of Basic Atomic Characteristics. Pilania etc. [40] will be effective features The search strategy is combined with state-of-the-art statistical learning methods to propose A method based on kernel ridge regression (Kernel Ridge Regression) Statistical learning model and a simple set of element descriptors, using To effectively predict the electronic band gap of double perovskites, the overall workflow.

In addition, Takahashi et al. [41] used random forest-based classification ML The model classifies the band gaps of perovskite materials. This model has a total of Used 18 physical descriptors used to classify a given perovskite material Whether the material is within the ideal band gap range (1.5~3.0 eV), and successfully Filter 15000 perovskite data and use DFT Calculate further Analyze stability step by step.

3.3 Lithium Battery Materials

Electric transportation and smart grid are the need of the times, lithium Ion batteries have high energy density, long life, low self-discharge and no Memory effect, as the most widely used energy storage device, plays an important role To function [42-43]. In order to ensure the smooth and reliable operation of the battery system, Accurately predicting the health of lithium-ion batteries (LIBs) is critical. However, battery degradation is a complex challenge involving the anode, separator The many electrochemical reactions at the membrane, cathode, and electrolyte / electrode interface answer. In addition, operating conditions also have a significant impact on battery degradation. Head Former various ML Techniques have been applied to estimate LIBs capacity and health to ensure reliable operation and timely maintenance.

An electrolyte is the medium through which ions migrate between electrodes (its activity called ionic conductivity), in order for the lithium ions in the liquid electrolyte To maximize conductivity, the solvent solubility of the lithium salt needs to be maximized ization and lithium ion viscosity are minimized. Sodeyama Wait [44] to match Bit able and melt point do for refer to mark,Test inspect Got it many Yuan Wire Sexual return return (MLR), least absolute shrinkage selection operator (LASSO) and linear regression Exhaustive search (ES - LiR) 3 Estimation accuracy and

effectiveness of information technology rate, found using ES - LiR Liquid electrolysis can be predicted more accurately The solvation energy and melting temperature of the liquid solvent; electrolyte additives can help expand the voltage range. The additives dissociate and react in the electrolyte during the initial stage of (discharge) charging. In liquid electrolytes and A stable solid electrolyte interface layer is formed between the electrodes [45]. Ok moto and Kubo [46] used a regression model to predict the performance of molecular additives. Oxidation potential; lithium ion migration barrier is widely calculated as a surrogate measure of ionic conductivity. Jalem et al [47] applied partial least squares Algorithm predicts olivine type LiMXO 4 migration barrier, and proposed New promising olivine-type solid electrolytes; lithium ion migration Trajectories have also been widely studied, Chen et al. [48] developed a cryptographic degree clustering method to elucidate the lithium migration of garnet-type solid electrolytes Move trajectory.

For electrodes, lithium ions are intercalated and deintercalated in the electrode to store Store and release energy. Embedded properties of electrodes are important for energy and power Density matters, number of parameters involved in electrode manufacturing process and the complexity of physical and chemical interactions throughout the associated processes properties, making the relationship between electrode characteristics and manufacturing parameters change It's very complicated. The electrode manufacturing process also strongly affects LIB special Properties, electrode slurry properties and coating parameters are the main factors affecting electrode heterogeneity, thereby affecting battery performance and life. To achieve high energy density, researchers focus on understanding structure by controlling the elements and structure of electrode materials -Performance relationship. Cunha etc [49] Analyzes 3 kind of different ML algorithms (decision trees, support vector machines and deep neural networks), The aim was to find the best algorithm to reveal the interdependence between slurry manufacturing parameters and the final performance of nickel manganese cobalt (NMC)-based cathodes. The results show that the support vector machine method has high accuracy and can predict the influence of manufacturing parameters on electrode mass loading and porosity in an intuitive and graphical manner.

LIBs of sex able exist very big Procedure Spend superior also Pick decide Yu Dian pool temperature degree, especially in terms of battery aging and safety issues. in low temperature bar Under conditions, due to reduced reaction kinetics, the availability of lithium is reduced, so There is a risk of lithium plating. However, operating at high temperatures LIBs possible Can lead to an increase in adverse side effects and rapid degradation, including quantity and power loss [50]. Ströbel et al. [51] proposed a method based on electrochemical Learn impedance spectroscopy and artificial neural networks LIBs Sensorless temperature estimation calculation method, by using the data of 28 cells to train the neural network network, and estimate the same cell type 8 The cell temperature of more than one cell Degree, neural network (a simple feedforward neural network with only one hidden layer The estimation accuracy that can be achieved through the network is $\Delta T = 1 \text{ K}$ ($10 \text{ }^\circ\text{C} < T < 60 \text{ }^\circ\text{C}$, T is the temperature) and the calculation amount is small.

3.4 Hydrogen Fuel Cell Materials

As one of the most promising energy sources, hydrogen energy has It will not produce carbon-based emissions and has abundant sources [52-53]. In response to various Environmental energy issues such as global warming, fossil fuel depletion, energy shortage It plays a huge role in shortage and pollution [54-55]. In order to better utilize hydrogen energy, proton exchange membrane fuel cells (PEMFC) have received great attention research attention. As an efficient electrochemical energy conversion device, PEMFC Can convert chemical energy in hydrogen into electrical energy and hot able, none need burn burn and null gas Sewage dye thing zero Row Put [56]. and and PEMFC It has the advantages of high power density, fast start-up, low operating temperature and portability [57], and also has wide application in vehicle power supply. Applications.

PEMFC uses polymer electrolyte membranes (such as Nafio n membrane) comes Conduct protons and separate gaseous reactants on both sides of the anode and cathode, Membrane electrode assembly (MEA) performance is important for PEMFC Very heavy Want [58]. Such fuel cells require expensive electrocatalysts (usually Platinum-based materials) catalyze electrochemical reactions at low temperatures. at present PEMFC The two main barriers to worldwide adoption are durability performance and cost, and advances in materials, operational controls and design are critical to reducing costs and improving durability.

Study on the synthesis of low-cost, high-activity and high-stability platinum-based materials Catalyst for PEMFC The large-scale commercialization of righteous. Liu Waiting for training on the experimental data set in our own laboratory 9 kind different ML Algorithm, for ionomer / catalyst ratio, water content, Organic solvents, catalyst loading, stirring method, solid content and ultrasound Spray flow rates are optimally selected to accurately predict performance and Pt Utilization rate, successfully achieving ultra-low single-cell battery Pt load [59]. Mai [60] prepared carbon-supported platinum-cobalt nanoparticles (NPs) using the impregnation reduction method for oxygen reduction reaction (ORR). By changing the heat treatment temperature, it is possible to control Pt3Co Structure, crystal phase and size of nanoparticles inch, and pure Pt Compared to Pt consumption is reduced and due to its smaller Particle size and higher alloying degree, the most stable among all samples good. combined with further DFT Calculations show that high alloying degree Pt3Co The structural surface can reduce the speed-determining step barrier and improve ORR live sex. In addition, a variety of processes will occur during the operation of the fuel cell. Interrelated and complex phenomena including mass / heat transfer, Electrochemical reactions and ion / electron conduction, these phenomena determine the energy Quantity conversion and efficiency.

ML exist PEMFC Modeling has the unique advantage that it does not require Prior knowledge is required, especially PEMFC Complex current transmission in operation transmission and electrochemical processes, greatly reducing the difficulty of modeling. ML, base of physical D.L. and AI Can promote basic knowledge relevancy, materials Choices and Advances, Fuel Cell Design and Optimization, System Control, Electricity Developments in source management and operational health monitoring, advancing PEMFC The technology aspect shows great potential. for catalyst Optimization, Zhu et al. [61] combined DFT calculation and ML to effectively filter out improved ORR Active Bimetallic Catalyst (DMSC) performance. they carried out DFT Calculated to predict a range of catalysts, these features are simplified, retaining the most relevant ones for the database, and trained ORR Fitting equation between activity and catalyst properties. Maohe Jackson [62] in PEMFC voltage and health status Artificial neural network, Adaptive neuro-fuzzy inference System (ANFIS) and Particle Filter (PF) methods. The results show, ANFIS provides accurate predictions at low computational cost, and PF Suitable for complex situations such as fuel cell failure. Ma Wait [63] to use Grid Long Short-Term Memory (G-LSTM) RNN A novel data-driven approach for degradation prediction developed D.L. Model. with traditional neural nets Compared with the network, this model effectively avoids gradient explosion and optimizes the prediction Measurement accuracy. and gives the complete G- LSTM RNN training algorithm, Including forward propagation of each neuron output, backward propagation (timeline or network layer) of error of each neuron, according to the corresponding error The difference term calculates the gradient of each weight and updates the weights through stochastic gradient descent. Its structure is simple and easy to implement online, and when combined with When used in combination with appropriate control strategies, can be used to improve durability, Efficiently achieve high prediction accuracy under various fuel cell operating conditions Spend.

Chen et al. [64] combined the particle swarm optimization algorithm (PSO) and the moving window method to propose a gray neural network model (GNNM). The model takes into account current density, inlet temperature, inlet hydrogen pressure and the effects of inlet relative humidity to better predict degradation under various operating conditions. Over time, due to the Nitrogen crosses over and liquid water accumulates, and battery performance will degrade. Efficient forecasting The short-term degradation behavior of proton exchange membrane fuel cells also has important significance. Yang [65] respectively adopted a method based on multivariate polynomials Regression (MPR) and A data-driven degradation prediction method for ANN, working flow Procedure, and carry out Got it one kind Knot Together with MPR and ANN 's M-ANN method. where V is the pressure, P is the pressure, t is time, I (t) is current density. use MPR predicts the initial value of battery performance I (1) and then use ANN Predict battery performance over time changes to describe PEM Degradation behavior of fuel cells. use DEA Proton exchange membrane fuel cell and anode recirculation in mode The model was trained on two degraded data in the model, which verified the effectiveness of the proposed method. The results show that the mean predicted by this method Average relative error ratio using only artificial neural network or MPR predicted flat The relative errors are much smaller. Predictive performance of two hidden layer neural networks Significantly better than a hidden layer neural network.

3.5 Thermoelectric Materials

With the decrease of natural resources, the development of alternative energy sources has increasingly become the focus of attention [66]. Thermal energy is a ubiquitous and abundant energy source that can be directly converted into electrical energy. Therefore, efficient utilization of thermal energy, such as waste heat recovery and solar thermal power generation, is essential to achieve a sustainable society in the future [67-68]. Traditional thermoelectric devices have complex structures and high manufacturing costs, making them difficult to deploy and use. Currently, thermoelectric technology based on the Seebeck effect has been regarded as a central approach to sustainable development [68]. This type of thermoelectric conversion can produce a new class of cheap and versatile thermoelectric devices [69]. A schematic diagram of the basic components and module structure of a thermoelectric device based on the Seebeck effect and the longitudinal spin Seebeck effect (LSSE), and a schematic diagram of the LSSE device structure being developed for future thermoelectric applications [70].

a fundamental mechanism for the spin Seebeck effect (SSE) and control SSE understanding of material parameters, device development has been influenced by hinder. ML Methods are becoming an indispensable tool for learning materials tools, statistical modeling and ML A data-driven approach to uncover hidden connections relationship and correlation [71-72]. Iwasaki et al. [73] used decision tree regression (DTR), elastic sex network Network (EN), two Second-rate many item Mode set So (QP- LASSO) and neural network (NN) which 4 types of supervised ML Model to establish control STE key physical parameters, and the number of descriptors The amount is fixed to 4 one, that is Δ a, n R, S R and L R. By predicting materials Iwasaki [73] also successfully developed a spin-driven thermoelectric material, and the thermoelectric potential of this thermoelectric material was uniform. Higher than all thermoelectric materials on the market today.

Thermoelectric ceramics are attracting attention for their potential to convert waste heat into electricity. It has aroused widespread interest among people [74-75]. Abdellah i et al [76] tried to adopt Adaptive Neuro-Fuzzy Inference System (ANFIS) (main component are fuzzy sets, fuzzy logic and neural networks) from Y content, compact Process parameters such as pressure, sintering temperature, sintering time and process temperature to make sure Sr 1- x Y x TiO 3 thermoelectric ceramic properties and the feasibility of the model Predictive evaluation to determine the dimensionless thermoelectricity of thermoelectric ceramics Excellent value,

3.6 Electrolysis of Water and Sodium Borohydride Hydrogen Production Catalyst

The key to electrolyzing water and sodium borohydride to produce hydrogen is the catalyst. Find low overpotential, excellent hydrogen evolution performance, and high hydrogen production rate [77-79]. To achieve this goal, this research group designed an AI Technical materials Model method for classification and classification of material synthesis parameters. The main steps are: converting the catalytic performance Y of the material as target letter number, determine the parameters that need to be optimized X With the range ($i = 1, 2, \dots, n$, a, b are constants), test the performance of the material Y_N through experiments ($N = 1, 2, \dots, n$), which can be divided into sensitive parameters and insensitive parameters. In the sensitive parameters, each parameter is divided again through the hierarchical formula n point are first-level, second-level, and third-level parameters. According to the numerical point and period of the parameter, Compare and analyze the numerical spread value of the edge with the threshold to determine how Next step is optimization. This model method was used in the optimization process of electrolysis of water and sodium borohydride hydrogen production catalyst materials, and through multiple experimental experiments According to the certification, the experimental synthesis parameters were classified and hierarchically optimized, and the catalytic performance of the material was quickly optimized. through experimental parameters A hierarchical classification model can be prepared after optimization through a limited number of experiments. New materials with high catalytic activity have effectively improved the research and development of catalyst materials. It improves development efficiency and realizes intelligent optimization management of parameters during the experiment. In order to further realize the automation of solution configuration and intelligent data processing, finally realized AI Experimental optimization of the preparation of new materials lays the foundation for research and provides new research ideas for the development of such materials.

4 SUMMARY AND OUTLOOK

artificial intelligence Advances in technology and further developments in computational materials science, It has brought new ideas and methods to the research and development of materials, subverting the Existing materials research model. D.L. and new technologies such as high-throughput computing It provides a new means to improve the efficiency of material research and development, which can Enough to significantly reduce the repetition, trial and error in the material development process work, significantly shortening the research and development cycle and accelerating theoretical innovation in the development of new materials. Currently, A.I. The application of technology is no longer limited to the discovery of new materials at the theoretical level, but also the further utilization of Use in-situ characterization and other technologies to conduct autonomous experiments and preliminary explorations and predict the theoretical parameters of new materials, and can also form a closed-loop reaction Feedback mechanism, through continuous learning and optimization, independent rapid iteration, improve High prediction accuracy.

In terms of materials research and development, AI Technology can often only target specific A certain material or type of material is subjected to high-speed, Autonomy Chemical research has limitations and cannot completely replace manual labor. at present Look, for materials and performance research and development AI There are many algorithms, but There are very few interpretable theoretical models, so in the future this field will expand the number of Starting from database and accessibility, we implement AI material for theoretical guidance Material experiment synthesis characterization test, making full use of the collaboration between experiment and theory The same effect can be achieved in materials science, chemistry and computer science. Subject development, through scientific researchers proving feasibility and finally putting it into industry change.

COMPETING INTERESTS

The authors have no relevant financial or non-financial interests to disclose.

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