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Trend Analysis on the Construction of AI-Based New Material Synthesis Processes and Process Optimization

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Abstract: *Traditional new material synthesis predominantly adopts an empirical trial-and-error R&D model, which suffers from deficiencies such as insufficient standardization of process flows, complex parameter coupling mechanisms, prolonged development cycles, and poor preparation stability, making it difficult to meet the demands of high-end new materials for efficient, green, and large-scale industrial production. Artificial intelligence technology provides crucial support for the paradigm innovation of material R&D, effectively breaking through the developmental constraints of traditional synthesis processes. This paper focuses on AI-powered intelligent synthesis of new materials, conducting a comparative analysis of the paradigm differences between traditional and intelligent synthesis approaches. It establishes a comprehensive intelligent synthesis process system for new materials, integrating data processing, intelligent modeling, path design, parameter optimization, closed-loop verification, and process standardization. Centered around five application scenarios—formula optimization, dynamic parameter regulation, streamlined green processes, defect tolerance management, and mass production process adaptation—the study systematically outlines the application pathways of AI in optimizing synthesis processes. Additionally, it identifies existing bottlenecks in intelligent synthesis technology regarding data, models, engineering implementation, and industry standards, while forecasting future trends in technology, industry, and the industrial ecosystem. The research clarifies the development direction of intelligent synthesis technology, offering theoretical reference for the intelligent R&D of new materials and the industrialization upgrade of processes.*

Keywords: *artificial intelligence; new material synthesis; process construction; process optimization*

1. Introduction

New materials serve as the core foundation for strategic emerging industries such as high-end equipment, new energy, electronic information, and biomedicine, and are a key indicator of a nation's high-end manufacturing and technological innovation capabilities. With accelerated industrial upgrading, the market has raised higher demands for the performance precision, preparation efficiency, green low-carbon properties, and batch stability of new materials[1]. Traditional new material synthesis models, centered on researchers' experience and reliant on extensive repetitive trial-and-error experiments, suffer from inherent flaws such as prolonged R&D cycles, blind parameter regulation, high energy consumption costs, and poor process replicability, which constitute a major bottleneck hindering the industrialization of new materials[2]. The deep integration of artificial intelligence and materials science drives the transformation of material R&D from an "experience-driven" paradigm to a new model of "data-driven, intelligent decision-making, and closed-loop iteration." This advancement can break through the dimensional limitations of traditional experiments, precisely uncover the intrinsic correlations between synthesis parameters and material performance, as well as reaction mechanisms, and significantly enhance the efficiency of new material R&D and production. Against this backdrop, systematic research on AI-enabled methods for constructing new material synthesis processes and optimizing trends holds significant theoretical and engineering value for promoting the intelligent upgrading of materials science and accelerating the industrialization of new materials.

Advanced countries such as those in Europe, America, and Japan have taken the lead in establishing AI-driven intelligent R&D systems for materials, setting up autonomous driving material laboratories[3]. Leveraging high-throughput experimentation, large-scale model retrosynthetic design, and real-time reinforcement learning regulation technologies, they achieve rapid synthesis and process iteration of various new materials, building comprehensive standardized material databases and algorithm systems,

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and implementing large-scale intelligent synthesis applications[4]. In China, supported by the dual strategies of new materials and artificial intelligence, phased achievements have been made in areas like formulation prediction, parameter optimization, and pathway screening. However, issues such as fragmented data, low process standardization, insufficient algorithm industrial adaptability, and an incomplete closed-loop system persist, leaving industrialized intelligent synthesis applications still in their infancy.

This paper focuses on the core issues of constructing AI-driven new material synthesis processes and intelligent optimization of processes, with the main research content being the development of a comprehensive technical framework for AI-enabled new material synthesis, analyzing key application scenarios for AI process optimization, identifying current technical bottlenecks, forecasting future industry trends, and proposing development strategies. The technical approach follows a research logic of "literature review—framework construction—application analysis—problem analysis—trend forecasting—conclusion." The primary innovation of this study lies in establishing a standardized, fully closed-loop AI new material synthesis process system, systematically defining the process scenario compatibility logic of various AI algorithms, and multidimensionally predicting the industrialization development trends of intelligent synthesis technology by integrating academic and industrial perspectives.

2. Fundamentals of AI new material synthesis technology and construction of the whole process system

2.1 Defects in traditional synthesis processes and the transformation of intelligent synthesis paradigms

The traditional new material synthesis system relies on the experimental experience accumulated by researchers to carry out research and development, which includes core processes such as raw material screening, component allocation ratio, reaction condition regulation, sample post-treatment, and performance testing and verification. This mode highly relies on manual trial and error and subjective experience judgment, and has not yet formed a unified and standardized operating system, resulting in poor controllability of the synthesis process [5]. In the actual research and development process, there is a strong coupling relationship between multidimensional process parameters such as temperature, pressure, reaction time, and composition ratio. Traditional experimental methods are difficult to accurately analyze the synergy and constraint mechanisms between parameters, and cannot precisely lock in the optimal process window. At the same time, human led trial and error R&D has poor repeatability, strong randomness, and is prone to problems such as large experimental result dispersion and insufficient batch stability. This not only significantly prolongs the development cycle of new materials, but also causes a large loss of reagents, equipment, and labor costs, making it difficult to adapt to the modern preparation needs of high-precision, customized, and batch production of high-end new materials [6]. Compared with the traditional R&D model, the AI driven intelligent synthesis paradigm has achieved fundamental innovation, relying on massive experimental data mining, high-precision intelligent modeling, and closed-loop iterative optimization capabilities, completely breaking through the technical limitations of traditional trial and error R&D, and forming significant advantages in R&D cycle compression, cost control, parameter control accuracy, process stability, and replicability. It has built a new material R&D paradigm that is data-driven, active design, dynamic iteration, and precise optimization.

2.2 Core AI technology system for intelligent synthesis of new materials

The technology system of AI enabled new material synthesis has high adaptability and pertinence. Various algorithm models form a layered application system based on the characteristics of material synthesis scenarios, forming the core technology foundation for intelligent process construction and process optimization [7]. Among them, graph neural networks can accurately adapt to modeling the microstructure characteristics of materials, effectively capturing the intrinsic correlation between atomic and molecular topological structures and material properties, and are suitable for predicting and designing new material structures; Bayesian optimization has excellent small sample iteration ability, which can efficiently optimize process parameters under limited experimental samples and adapt to the industry characteristics of scarce samples in new material research and development; Reinforcement learning can rely on real-time feedback of working conditions to achieve dynamic decision-making, meeting the multi-stage and dynamic process control requirements of the synthesis process; The big language model can deeply mine the implicit synthesis knowledge in massive literature, patents, and

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experimental data, realizing the sorting of synthesis paths and intelligent generation of process plans; Generative AI focuses on material inverse synthesis design, which can deduce the optimal synthesis scheme based on target performance and broaden the boundaries of material research and development; Explainable AI effectively solves the "black box" problem of traditional intelligent models, achieves model decision traceability and parameter mechanism visualization, and enhances the scientific and credibility of process optimization results[8].

2.3 AI driven framework construction for the entire process of new material synthesis

Based on the application characteristics of various AI technologies, this article constructs a modular, standardized, and closed-loop iterative new material intelligent synthesis full process system, forming a multi-level collaborative complete R&D chain. This system mainly covers six core levels, each level performing its own duties and iterating in a coordinated manner. The data layer integrates high-throughput experimental data, simulation calculation data, and literature structured data to complete data cleaning, normalization, and standardized labeling, and constructs a high-quality material synthesis dataset; The modeling layer integrates data features and material physical and chemical mechanisms to construct a coupled correlation model of "process parameters microstructure macroscopic performance", enhancing the model's generalization ability and physical rationality; The design layer relies on generative AI to optimize formula components and reverse plan synthesis pathways, achieving goal oriented active design [9]; The optimization layer is based on multi-objective intelligent algorithms, taking into account constraints such as performance, cost, and energy consumption, to achieve global optimization of process parameters; Establish a closed-loop iterative mechanism of "AI design simulation prediction experimental verification model iteration" in the verification layer to continuously correct model deviations; The output layer modularizes and standardizes the archiving of mature synthesis processes, achieving cross scenario reuse and industrial implementation of high-quality processes. As shown in Figure 1.

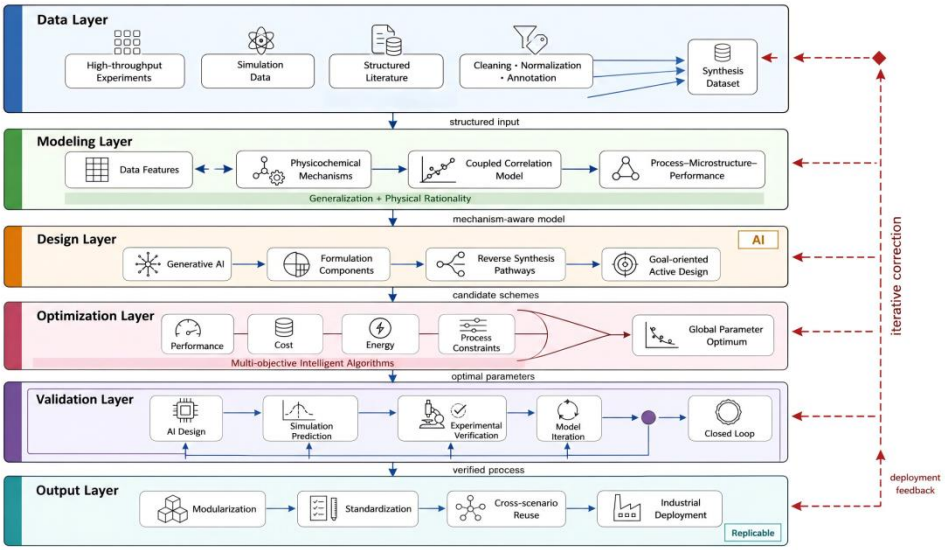

Figure 1. AI driven modular closed-loop system framework for the entire process of new material synthesis

3. Core application scenarios of AI in optimizing new material synthesis processes

3.1 Intelligent optimization of formula system

The material formula is the core basis for determining the microstructure and macroscopic properties of new materials[10]. Traditional formula optimization relies on univariate control experiments, which can only achieve simple tuning of a limited number of components and cannot analyze the synergistic and antagonistic effects between multiple components. It is prone to problems such as formula redundancy, limited performance limits, and high raw material costs. AI technology, relying on machine learning, graph neural networks, and generative models, can achieve intelligent screening, feature analysis, and precise iteration of multi-component, high-dimensional formulation systems, and build a

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new paradigm of formulation design driven by performance goals in reverse. By mining the features of massive experimental data, literature data, and high-throughput simulation data, AI models can accurately identify the core influence weights of matrix materials, doping components, and functional additives, eliminate invalid redundant components, mine the optimal ratio relationship of multiple components, and break through the empirical limitations of traditional artificial formulas. At the same time, generative AI such as variational autoencoders and diffusion models can reverse engineer new candidate formulation systems based on target mechanical properties, electrochemical properties, optical properties, and other indicators, greatly expanding the design space for new material formulations. In the fields of energy storage materials, composite materials, optoelectronic materials, etc., AI formula optimization can effectively improve the core performance of materials, reduce the amount of valuable raw materials, significantly reduce research and development and production costs while ensuring material stability, and achieve efficient, refined, and low-cost upgrading of the formula system. As shown in Figure 2.

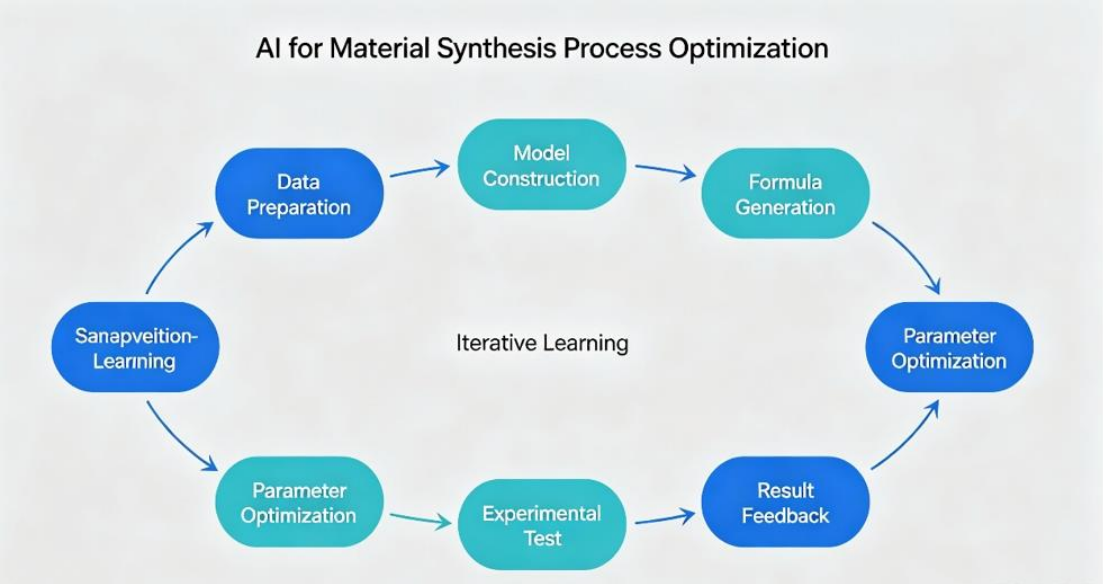

Figure 2. Intelligent optimization of formula system

3.2 Precise control of dynamic process parameters

The synthesis of new materials is a typical dynamic nonlinear reaction process, in which process parameters such as temperature, pressure, reaction time, stirring rate, heating rate, and material flow rate are coupled and dynamically changed. The traditional fixed parameter control mode cannot adapt to the real-time evolution law of the reaction system, which can easily lead to the growth of side reactions, the generation of micro defects, and batch performance fluctuations. A dynamic control system based on AI algorithms such as reinforcement learning and Bayesian optimization can achieve real-time perception, dynamic correction, and precise optimization of parameters throughout the synthesis process. The AI model constructs a real-time correlation model between process parameters, reaction states, and material properties by collecting dynamic data such as spectra, temperature fields, and pressure fields during the synthesis process. It adaptively adjusts process parameters based on the evolution characteristics of different stages of the reaction, accurately matching the laws of reaction kinetics and thermodynamics. Compared with traditional static parameter control, AI dynamic control can accurately lock the optimal process dynamic window, effectively suppress side reactions, improve reaction conversion rate and raw material utilization, solve the pain points of poor batch consistency and low yield rate in traditional processes, greatly improve the stability and controllability of new material preparation, and adapt to the precise synthesis needs of high-precision nanomaterials, thin film materials, and catalytic materials.

3.3 Simplification and green optimization of synthesis processes

Traditional new material synthesis generally suffers from problems such as complicated processes, redundant processes, high energy consumption, and large pollutant emissions. The preparation process of some complex materials includes multi-level reactions, repeated post-treatment processes, long research and development cycles, and serious resource consumption, which does not conform to the

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green and low-carbon development trend of the materials industry. By relying on big language models and knowledge graph technology, AI can deeply explore massive synthesis literature, patent processes, and industrial cases, sort out the energy consumption, efficiency, and environmental characteristics of different synthesis paths, and achieve intelligent simplification and process reconstruction of synthesis processes. The AI system can accurately identify redundant processes, invalid operations, and high-energy consumption links, optimize process connection logic, merge duplicate processing flows, and screen out the optimal synthesis path with short processes, low energy consumption, and low emissions. At the same time, through multi-objective optimization algorithms, a green process optimization model that balances synthesis efficiency, preparation cost, and environmental indicators is constructed to shorten the preparation cycle, reduce energy consumption, and minimize waste liquid and residue emissions while ensuring that material performance does not deteriorate. This optimization mode effectively addresses the shortcomings of traditional processes that prioritize performance over green, and promotes the iteration of new material synthesis processes towards high efficiency, lightweight, and green direction, which is in line with the high-quality development requirements of the new material industry under the dual carbon background.

3.4 Defect prediction and process fault-tolerant optimization

During the synthesis process of new materials, micro defects such as pores, cracks, agglomeration, and component segregation are easily generated. The random generation and difficulty in predicting defects are key challenges that restrict the yield and performance stability of materials. Traditional defect control relies on post inspection and process review, which has problems such as strong lag, high treatment costs, and poor fault tolerance. AI technology can achieve pre prediction, in-process intervention, and post traceability of synthetic defects, and build a fault-tolerant optimization system for the entire process. By using convolutional neural networks and time-series prediction models to conduct in-depth analysis of synthesis process parameters and reaction environment data, AI can accurately identify the core causes of defect generation, establish a correlation prediction model between "process anomalies and defect generation", and predict high defect incidence conditions and key nodes in advance. Based on the predicted results, the model can adaptively optimize process parameters, adjust operating standards, and avoid the risk of defect generation; For generated defects, process vulnerabilities can be located through feature tracing, iterative optimization of process fault tolerance mechanisms, and improvement of the anti-interference ability of the synthesis process. This technological system has completely changed the traditional passive governance mode of "defect first, rectification later", significantly improving the qualification rate and performance consistency of new material preparation, and providing technical support for the stable preparation of high-precision functional materials.

3.5 Optimization of industrial mass production process adaptation

The optimal laboratory process generally faces the challenge of scaling up. The differences in operating conditions, heat and mass transfer effects, and material batch differences from small-scale and pilot scale to mass production can easily lead to process failure, performance degradation, batch fluctuations, and other amplification effects, which are the core barriers that restrict the industrialization of new material research achievements. Traditional craftsmanship relies on manual experience for debugging, with long iteration cycles, high trial and error costs, and poor adaptability. AI technology can accurately fit the differences in working conditions of different preparation scales, achieving industrial adaptation and iterative optimization of laboratory processes. By constructing multi-scale process datasets for small-scale, pilot scale, and mass production, AI models can analyze the parameter offset patterns, error accumulation mechanisms, and performance degradation mechanisms during the scaling up process, and optimize the mass production process parameter system, equipment operating parameters, and production control standards in a targeted manner. At the same time, combined with the multiple constraints of industrial production, multi-objective collaborative optimization of mass production processes is carried out to balance production efficiency, product quality, production costs, and production stability, effectively solve the problem of process amplification, break through the technical barriers of "laboratory research and development industrial mass production" of new materials, greatly improve the transformation efficiency of scientific research achievements, and promote the intelligent synthesis process from laboratory demonstration to large-scale industrial application.

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4. Existing bottlenecks and industry development trends

4.1 Current AI new material synthesis technology and industry bottlenecks

From the perspective of technology and industry implementation status, there are still many bottlenecks that urgently need to be overcome in the current AI enabled new material synthesis system. Firstly, there are structural defects in the data system, such as data fragmentation, low standardization, and severe data silos in the field of material synthesis. The existing public datasets mostly focus on successful experimental cases, with a large amount of missing failed experimental data and invalid parameter data, resulting in sample bias in model training, making it difficult to fully cover the process evolution laws under complex working conditions, greatly reducing the generalization ability and robustness of intelligent optimization models. Secondly, there are problems with the lack of mechanism and interpretability in algorithm models. Currently, mainstream intelligent optimization models are mostly purely data-driven models, overly relying on sample data fitting and failing to fully integrate material thermodynamics and kinetic reaction mechanisms. The model output results often lack physical and chemical support, and there are problems such as insufficient rationality of optimization parameters and poor adaptability to extreme working conditions. At the same time, AI models generally have "black box characteristics", making it difficult to trace the process of process optimization decision-making and effectively explain the intrinsic mechanism of parameters and performance, which limits their practical application in high-precision industrial scenarios.

In addition, the shortcomings of project implementation and industry adaptation are prominent. At present, most intelligent synthesis algorithms and optimization frameworks are developed based on ideal laboratory conditions, without fully considering complex factors such as equipment errors, environmental disturbances, and batch fluctuations in industrial production. The optimal laboratory process is difficult to directly achieve large-scale reuse. At the same time, the cost of intelligent synthesis supporting equipment is high, the degree of automation integration is insufficient, and most enterprises lack intelligent research and development and production systems, resulting in a low penetration rate of AI process optimization technology industrialization. Finally, the industry standard system is not yet sound, and there is currently no unified material synthesis data annotation standard, model evaluation standard, and process optimization evaluation system in China. There is a lack of unified standards for technology research and development and implementation, and the industry development presents fragmented and disorderly characteristics, which restricts the large-scale promotion and industrialization iteration of technology.

4.2 Technological development trends

The future AI new material synthesis technology will continue to evolve towards mechanism fusion, high interpretability, and fully closed-loop autonomous iteration. Firstly, the coupling model of data-driven and mechanism constrained fusion will become the mainstream development direction. By embedding material reaction mechanisms and physical and chemical rules into AI algorithm frameworks, the theoretical deficiencies of pure data models will be compensated for, and the scientificity and reliability of process optimization results will be improved, solving optimization problems in extreme working conditions and small sample scenarios. Secondly, interpretable artificial intelligence technology will be deeply implemented, gradually breaking the black box limitations of traditional models, achieving visualization of process parameter weights, traceable optimization decisions, and interpretable defect mechanisms, greatly enhancing the credibility and practicality of intelligent process systems. Thirdly, the fully automated closed-loop R&D system will continue to be improved, relying on material modeling, high-throughput experiments, and autonomous driving laboratory technology to achieve autonomous operation of the entire chain of "intelligent design simulation verification experimental preparation performance testing model iteration", completely changing the traditional segmented and fragmented R&D mode, and greatly improving the iteration efficiency of new material synthesis and process optimization.

4.3 Trends in industry and system development

At the level of industry and industry system, the intelligent synthesis of new materials will present a development trend of large-scale implementation, green upgrading, and standardized construction. On the industrial side, with the iteration of lightweight algorithms and the popularization of domestically produced intelligent devices, the landing cost of intelligent synthesis technology continues to decline,

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gradually penetrating from university laboratories and top research institutions to small and medium-sized enterprises. The collaborative transformation system of industry university research and application is constantly improving, effectively breaking down the barriers between laboratory research and industrial mass production, and realizing the large-scale industrial application of intelligent processes. At the same time, driven by the dual carbon target, AI process optimization will take into account performance, efficiency, and energy consumption and environmental protection indicators, forming a multi-objective collaborative green intelligent optimization system, and promoting the green and low-carbon transformation and upgrading of the new material synthesis industry. At the industry system level, a unified standard for material data collection, labeling, and sharing will be gradually established in the future, and a standardized system for AI model verification, process optimization evaluation, and achievement landing evaluation will be improved. A standardized, reusable, and traceable intelligent material research and development industry ecosystem will be constructed to continuously promote the high-quality development of China's new material industry towards intelligence, high-end, and scale.

5. Conclusion

This article takes the empowerment of artificial intelligence in the intelligent synthesis of new materials as the research mainline, systematically conducts research on the trend of synthesis process construction and process optimization, and clarifies the paradigm change logic, technical system architecture, and industrial application path of AI driven material research and development. Research has shown that the traditional research and development model for synthesizing new materials relies on experience trial and error, which has inherent shortcomings such as lack of process standardization, fuzzy parameter coupling mechanism, low iteration efficiency, poor batch stability, and weak industrial adaptability. It is difficult to adapt to the high-precision, green, and large-scale development needs of high-end new materials. Artificial intelligence technology, with its high-dimensional feature mining, nonlinear fitting, and multi-objective collaborative optimization capabilities, can effectively break through the technical limitations of traditional processes and promote the comprehensive transformation of material research and development from an empirical trial and error paradigm to a data-driven, closed-loop iterative intelligent paradigm.

This article constructs a modular AI new material synthesis full process system covering data layer, modeling layer, design layer, optimization layer, verification layer, and output layer, forming a reusable, iterative, and industrializable intelligent synthesis technology framework. At the same time, the system has identified the core application advantages of AI in five major scenarios: formula system optimization, dynamic parameter regulation, green and streamlined processes, defect tolerance management, and mass production process adaptation. It has clarified the important value of intelligent process optimization in improving synthesis efficiency, enhancing material properties, and reducing preparation costs.

The research further points out that there are still practical bottlenecks in the current field of AI new material synthesis, such as insufficient data quality, weak model interpretability, low degree of mechanism decoupling, poor industrial adaptability, and lack of industry standards. In the future, intelligent synthesis technology for new materials will evolve towards mechanism integration, interpretable modeling, and full chain automation closed-loop iteration. The industrial end will gradually achieve lightweight, low-cost, and large-scale implementation, and the supporting data standards, evaluation systems, and industry standards will continue to be improved, continuously promoting the high-quality transformation and upgrading of China's new material industry towards intelligence, greenness, and high-end.

References

[1] Linghu J J, Lei S, Liu H, Zhang Y, Han N N, Li Z P. Empowering New Material Design with Machine Learning: A Paradigm Change from Experience Trial and Error to Data Driven [J]. Computational Physics, 2026,43 (1): 2-20.

[2] Chen X, Song Z L, Lu S H, Wu Y L, Ju M G, Zhou Z H, Wang J L. AI driven material design: paradigm shift from small data to big data [J]. Chinese Science: Chemistry, 2025, 55 (6): 1648-1659.

[3] Liang C, Rou Z H, Ye C Y, Li C,Wang B, Li H S.Material symmetry recognition and property prediction accomplished by crystal capsule representation[J].Nature Communications, 2023, 14(1):5198-5198.

[4] Wang Z G, Wan M, Chen Z Y, Li K, Wang X G, Liu M, Meng S, Wang Y Q. Research and Application of Data Driven Material Intelligent Design Platform [J]. Frontiers of Data and Computing Development,

ISSN 2616-7433 Vol. 8, Issue 3: 1-8, DOI: 10.25236/FSST.2026.080301

2023, 5 (2): 86-96.
[5] Abolhasani Milad, Kumacheva Eugenia. The rise of self-driving labs in chemical and materials sciences[J].Nature Synthesis,2023,2(6):483-492.
[6] Malik Shreshth A., Goodall Rhys E. A., Lee Alpha A. Predicting the Outcomes of Material Syntheses with Deep Learning [J].CHEMISTRY OF MATERIALS,2021,33(2):616-624.
[7] Ren R Q, Zhao Z H. AI-assisted synthesis in reticular framework materials [J]. Journal of Capital Normal University: Natural Science Edition,2026,(3):49-60.
[8] Jiao L, Hua Y, et al. Current Status and Prospects of Resource Recycling Technology for Fiber-Reinforced Polymers in the New Energy Industry [J]. Energy Environmental Protection,2026,(1):28-41.
[9] Liu Z Y. Innovation and Application of Ammonia Separation and Purification Technology in the Process of Green Hydrogen Synthesis of Ammonia [J]. Shanxi Chemical Industry,2026,(2):213-215.
[10] Wu Y J, Li P X, et al. Research Progress and Challenges of Materials Genome Engineering and Intelligent Science in the AI+Era [J]. Foundry Technology,2026,(1):1-15.