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Review

A Review on Design of Sustainable Advanced Materials by Using Artificial Intelligence

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ABSTRACT: This paper gives a comprehensive review of scientific interests and current methodologies of artificial intelligence applied to advanced material design and discovery by taking into account multiple sustainable design criteria such as functionalities, costs, environmental impacts, and recyclability. The main research activities include predicting material properties, compositions, and structures with data mining, new material discovery, hybrid modeling approaches combining AI techniques and classical computational formulations based on physical and chemical laws, and multicriteria optimization of materials. Based on this review, a short analysis is provided on the perspectives of this research area in the future, aiming at creating an everything connected material life cycle with real-time traceability systems.

Keywords: Advanced material design; Sustainability; Artificial intelligence; Prediction; Hybrid modeling; Material discovery; Multicriteria optimization

1. Introduction

Advanced materials, which exhibit superior properties or functionalities compared to traditional materials, mainly include composite materials, smart materials, nanomaterials, biomaterials, advanced polymers, high-performance alloys, advanced ceramics, photonics materials, functional materials, and graphene 2D materials. These materials are urgently needed for various industrial areas and our everyday life. However, traditional ways of designing new materials encounter limits due to the complexity of physical and chemical compositions, structures, and targeted properties. Moreover, in the current situation, new materials should enable novel applications and include sustainable ways of producing, using, and recycling them [1]. This means that a new material design should consider comprehensive multicriteria optimization, i.e., minimizing environmental impact, promoting resource efficiency, and enhancing product functionalities and well-being for users throughout its whole lifecycle from sourcing and production to use and disposal.

In this context, artificial intelligence (AI) techniques have been widely used in the field of material science and engineering to discover, design, and optimize new advanced materials with sustainable features, i.e., enhanced functional properties, while considering other requirements. This involves using machine learning algorithms and computational methods to analyze vast datasets, predict material behavior, and accelerate the materials discovery process with multiple optimization criteria and accurate prediction capacities. Some specific key topics can be summarized from two review papers [2,3] as follows.

(1) **Prediction**: AI algorithms can analyze large datasets related to material properties, compositions, and structures to identify patterns of materials, correlations between technical design parameters and material performances. It also predictss new materials' properties using supervised and unsupervised data learning techniques.

(2) **Virtual Screening**: AI algorithms can be trained to predict the performance of materials and show them through static and dynamic simulations without extensive experimental testing. This enables researchers to virtually screen and prioritize potential materials from a large number of candidates for specific applications.

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(3) **Material Discovery**: AI algorithms can aid in discovering novel materials by suggesting new compositions or structures based on known data. This accelerates the process of finding materials with desired properties, such as improved strength, conductivity, or other functional characteristics.
(4) **Optimization**: Machine learning techniques can optimize material properties by suggesting modifications to existing materials. This may involve adjusting compositions or structures to achieve specific performance goals. Especially, multicriteria optimization criteria are usually used for identifying the most relevant material from a large number of candidates by using multiple criteria related to material sustainability, including improvement of material functionalities and recyclability, minimization of environmental impacts and costs.
(5) **Generative Design**: AI-driven generative design uses algorithms to explore and generate numerous design options. This is particularly useful in creating innovative material structures or configurations that may not be intuitive to human designers.
(6) **Knowledge base creation and updating**: The AI algorithms can to create a comprehensive material knowledge base by exploiting various materials' data. Researchers can exploit material properties and relationships from this knowledge base and update it by introducing new material design cases and relevant material data.

AI-based material design has attracted numerous researchers in various industrial areas. The number of annually published scientific papers on this theme indexed and collected in the database of Science Direct has increased 4.6 times over the last ten years (See Figure 1). This increasing trend has become especially important since 2020.

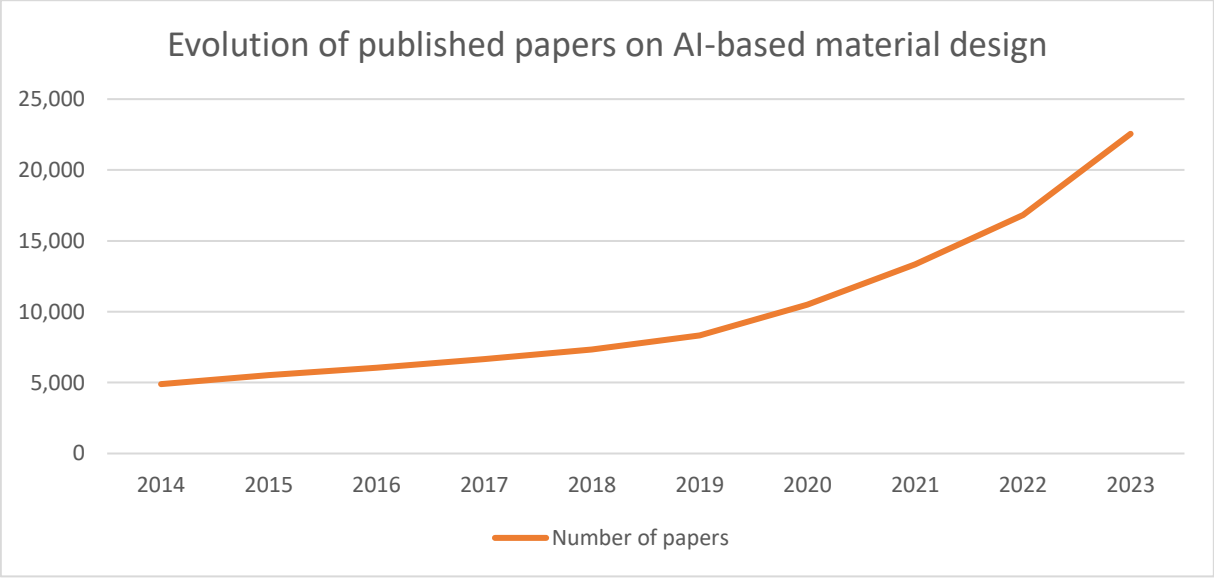

Figure 1. Evolution of published papers on AI-based applications in material science over the last 10 years.

It has been emphasized that the cooperation of AI and industrial simulation in sustainable material design represents a powerful synergy that can significantly enhance the efficiency and transparency of the materials design and development process. In practice, industrial simulations enable the generation of large amounts of data simulating the performance of materials in a digital environment under various conditions, in which designers can easily visualize the performance of materials and their future products. At the same time, AI algorithms can analyze the corresponding simulation results to predict trends and relationships that might not be immediately apparent to provide guidelines to designers for optimizing their design solutions in the real environment. In this context, an AI-based sustainable material/product design process will be created through a series of interactions between the AI functions and the interconnected design operations, i.e., the tools of modelling, data mining, knowledge engineering, optimization, prediction and simulation will be successively applied to the stages of design requirements identification, material structural determination, functional performance determination, technical parameters determination for material implementation, as well as prototyping, testing and new design knowledge exploitation. By using this process, the designers can realize the online monitoring of the material/product life cycle and online optimization of materials according to the decision support provided by the prediction results. The main principle of this AI-based design process is illustrated in Figure 2.

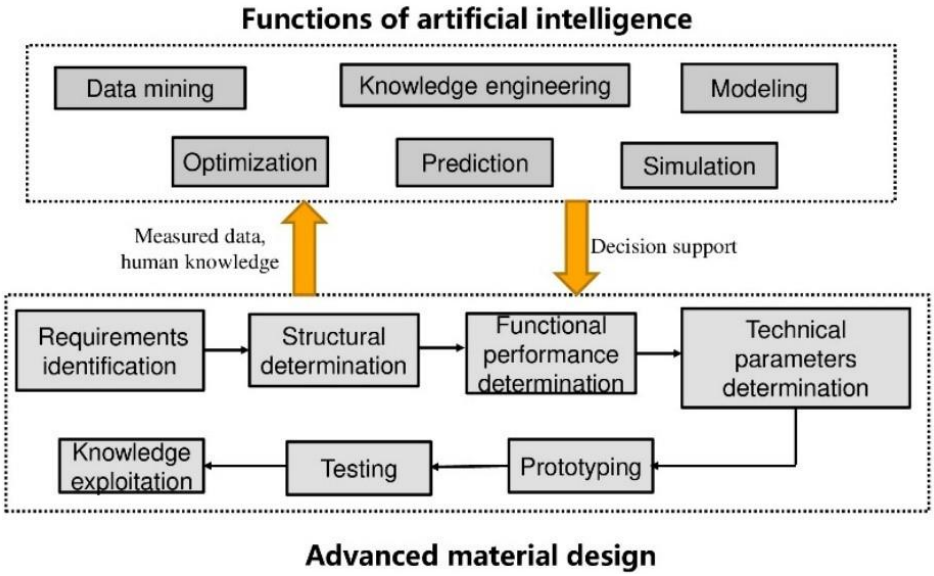

Figure 2. The general principle of the AI-based sustainable material design process: interactions between the AI functions and design environment.

The cooperation of physical-based models and AI techniques is another powerful synergy for advanced material design. Physical-based models, rooted in fundamental principles of physics and engineering, provide a solid foundation for understanding and simulating structures and functionalities of materials. These models can experience certain limits, regarding the quantitative prediction of high-dimensional phase equilibria and particularly the resulting non-equilibrium microstructures and properties. Moreover, many microstructure- and property-related models use simplified approximations and rely on a large number of variables. However, they often face challenges in accurately representing real-world complexities related to multiple scales and various compositions or accounting for uncertainties. In this situation, hybrid modelling approaches [4], combining machine learning and, deep learning and physical-based models, can effectively refine and improve the quality of classical physical models by learning from data and identifying patterns that might be uncertain and difficult to capture using traditional models only.

Researchers from the Max-Planck-Institut für Eisenforschung (MPIE) have reviewed the status of physics-based modeling and discuss how combining these approaches with artificial intelligence can open as-yet untapped spaces for the design of complex materials [3]. By using machine learning techniques, thermodynamic and microstructural features, key features can be automatically extracted from large data sets with high predictive power. However, as the predictive power of machine learning strongly depends on the quantity and quality of labelled data sets, ways of overcoming this obstacle are needed. One solution is to use active learning algorithms, in which machine learning models are initially trained with small sets of labelled data and then dynamically select the most informative data points to label according to predefined optimized searching strategies running in uncertain environments. This step-by-step approach leads to a final high-quality data set usable for accurate predictions. Another solution is to combine human knowledge discoveries and data mining-based approaches in a complementary way. In fact, data mining techniques excel at uncovering patterns and insights from large datasets, while human expertise provides context, domain-specific understanding, and intuition that can guide the data mining process and help interpret its results.

According to the analysis in [3], there are still many open questions regarding the use of artificial intelligence in materials design: How to handle sparse and noisy data; How to process multi-scale properties occurring in many materials; How to implement unwanted elemental intrusion from synthesis or recycling. Solving these problems requires the development of new AI solutions that are more adapted to the key features of material structures and functionalities and the integration of AI techniques and other computational tools, especially those dealing with classical physical laws.

This paper is organized as follows. Section 2 provides a systematic review of basic AI techniques frequently used in material engineering. They include not only data mining-based algorithms (supervised and unsupervised learning and reinforcement learning) but also human knowledge-based models (human engineering), their combinations (hybrid modeling) and multicriteria optimization. The advantages and drawbacks of each modeling approach will be discussed. The problems usually encountered in data mining, such as “overfitting,” will also be stated. This section selects the most well-known classical scientific books and journal papers on AI as theoretical foundations. By using these basic computational techniques, the applications in modelling and prediction of material structures, functionalities (especially

flows in porous structures), as well as multiscale material models and cooperation between modelling, simulation and optimization will be discussed in Section 3. The AI-based multicriteria or multi-objective optimization for material design will be stated in Section 4 in order to further optimize the material performance by considering all factors (material functionalities, costs and environmental impacts) comprehensively and in a balanced way, leading to the approaches of sustainable material design. The hybrid modelling approaches combining data-based models, human knowledge-based models and physical-based or chemical-based computational models in material design will be reviewed in Section 5. A conclusion will be given in Section 6. The references cited in the following sections have been preselected from the Science Direct Database according to various combinations of keywords on AI, material design and material performance. The AI keywords include AI, data mining, neural networks, deep learning, fuzzy model, knowledge model, expert system, multicriteria, optimization, and hybrid model. The material design keywords: material design and material structure. The performance keywords include functional, sustainable, environmental, mechanical, thermal and fluid. The preselected references have been further filtered based on the requirements of this paper.

2. Artificial Intelligence in Industrial Applications

Artificial intelligence is one of the leading disciplines in science and engineering and is concerned with all intelligence tasks. Currently, it covers numerous sub-areas, from generalized machine learning, reasoning and perception to specific topics, such as chess, mathematical theorem demonstration, poem composition, automatic car driving, and medical diagnosis. According to [5], AI mainly deals with four approaches: (1) **Thinking Humanly:** automation of human thinking (determining how human thinks: cognitive science); (2) **Thinking Rationally:** study of the computations that make it possible to perceive, reason, and act (determining laws of thought: logic); (3) **Acting Humanly:** art of creating machines that perform functions that require intelligence when performed by people (reasoning, knowledge representation and machine learning, computer vision, robotics); (4) **Acting Rationally:** study of the design of intelligent agents (making correct inferences to achieve the best outcome). A human-centered approach involves observations and hypotheses about human behaviors. A rationalist approach is a combination of mathematics and engineering. These approaches are complementary between them and can help each other. The problems involved in material design and discovery discussed in Section 1 mainly deal with acting humanly, including data mining based on physical measurements of materials, processes and environment and human knowledge representation and discovery from professional experiences.

2.1. Data Mining Approach

Data mining is a process to automatically discover patterns, trends, associations, or useful information from large-scale datasets. It is a subfield of machine learning. The primary goal of data mining is to extract valuable insights and knowledge from data, which may not be immediately apparent.

Data mining is usually composed of the following steps [6]:

(1) **Problem definition:** determining the goal of data mining and the problem to be solved.
(2) **Data collection:** collecting data on the problem from various sources: databases, documents, sensors and the Internet.
(3) **Data understanding:** making an exploratory analysis of collected data (statistics, data visualization, …) to understand their features, distribution and quality.
(4) **Data modelling:** selecting appropriate data mining techniques (classification, regression, clustering, association rules mining, …), in which data will be divided into training and testing datasets in order to evaluate the performance of the model.
(5) **Model training:** training the data mining model by using the training dataset, selecting the most relevant algorithm and adjusting parameters to optimize the model's performance.
(6) **Model evaluation:** evaluating the model's performance using the testing dataset with predefined indicators such as accuracy, robustness and F1 score.
(7) **Model optimization:** adjusting and optimizing the model (algorithm, features, …) according to the evaluation results.
(8) **Model deployment:** deploying the trained model to the real scenarios for applications.
(9) **Monitoring and maintenance:** monitoring the performance of the model and updating it for adaption to new coming data, and processing the problems of model drift and degradation
(10) **Interpretation and reporting:** explaining the results delivered from the model and giving suggestions on how to use them, and reporting the discovered results in numerical and visual form.

(11) **Feedback loop:** improving the data mining process according to the results and their feedback by introducing new problem definitions, collecting new data and using different modelling methods.

Data mining is an iterative process that usually requires continuous adjustment and improvement to achieve the best results. Data mining is a complex task, and the key issues to success lie in understanding the problem, selecting the right technique, and continuous experimentation and optimization. The most used data mining tasks include:

(1) **Supervised learning**, i.e., learning or setting up models from training datasets (pairs of input/output data or labelled data) for classification and regression. The essential problem in supervised learning is to select relevant models based on experimental data that is accurate, generalizable and interpretable without overfitting, i.e., the model learns the training data too well, to the point that it captures noise or random fluctuations in the data as if they were meaningful patterns (See Figure 3). The specific supervised learning methods are described below.

- **Linear Regression:** Setting up a linear relationship model between continuous input and output variables (e.g., house sales volume prediction).
- **Logistic Regression:** Dealing with binary classification problems and mapping input features to a probability value, commonly used for classification tasks.
- **Decision Trees:** Creating an easy to understand tree-like structure, commonly used to model decision-making processes involving linguistic variables and practically improved with pruning techniques to reduce overfitting [7].
- **Random Forests:** Combining multiple decision trees to enhance predictive performance and reduce overfitting by utilizing bootstrapping and aggregation (bagging). Random Forests have been widely used in prediction, classification and feature selection. They are considered one of the most efficient machine learning tools due to their high efficiency, robustness and capacity for big data processing [8].
- **Artificial Neural Networks (ANN):** Inspired by the biological neural system, ANNs are the most used supervised learning algorithm, designed for various tasks such as classification, regression, signal processing, time series forecasting, clustering, and more [9]. There are a large number of widely applied ANN models, including **Multilayer Perceptron (MLP)**, usually used to model continuous nonlinear relations; **Radial Basis Function Neural Network (RBF)**, which exhibit very good performances for regression when the training data have a clear cluster structure; **Recurrent Neural Network (RNN)**, specifically designed to handle time series and data with temporal dependencies with its special recurrent connections, allowing information to propagate within the network to capture historical information in time series; **Support Vector Machines (SVM)**, enabling to find the best hyper-plans for partition of training data.
- **K-Nearest Neighbors (KNN):** classification and regression based on neighboring data points, considering that neighboring data have similar labels.
- **Naïve Bayes:** computations based on Bayes Theorem for text classification and statistical estimation.
- **Convolutional Neural Networks:** Deep learning algorithms based on traditional ANNs, enabling the combination of feature extraction and supervised learning, which are specially adapted to deep learning tasks (i.e., performing complex tasks by learning from data without being explicitly programmed) such as image analysis and computer vision [10].

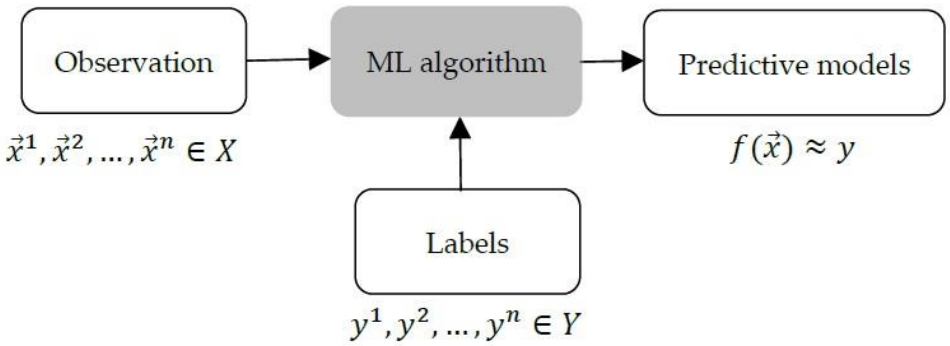

Figure 3. Principle of supervised learning.

(2) **Unsupervised learning**, i.e., discovering hidden structures or patterns from data, including clustering, dimensionality reduction, association rules mining, etc. Different from supervised learning, there is no data label in unsupervised learning. It involves modelling the raw data of the overall observations, particularly emphasizing

the modeling of the data's structure and correlations, without relying on external labels or supervised information, in order to better understand the intrinsic relationships within all the data (See Figure 4). This learning approach is commonly used to discover valuable information and patterns, such as identifying standardized quality metrics from a large amount of product data, extracting market segments from extensive sales data, or determining standardized human body dimensions from a large volume of human body data. Establishing a standard system based on raw data is the primary application area of unsupervised learning. The most common methods of unsupervised learning are clustering and Self-Organizing Maps [11].

- **Clustering:** Also known as grouping, aiming to partition the samples or data points in a dataset into different groups or clusters so that data points within the same group exhibit similarity while those in different groups have significant differences. The most used clustering algorithms include Hierarchical Clustering, K-Means and fuzzy C-Means.
- **Self-Organizing Maps (SOM):** One ANN model for data visualization and mapping high dimensional data to a lower dimensional space for clustering.

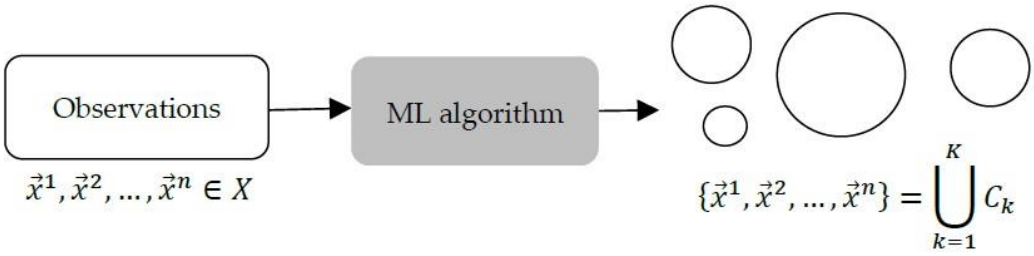

Figure 4. Principle of unsupervised learning.

(3) **Reinforcement Learning (RL)**, also known as semi-supervised learning [12]: Training agents to learn the optimal strategy through interaction with the environment, commonly applied to decision-making and control problems. Reinforcement Learning is a machine learning paradigm that teaches an agent to make decisions through interaction with the environment to maximize expected cumulative rewards. In RL, agents explore the environment by trying different actions and adjusting their behavior based on feedback from the environment (rewards or penalties) to achieve optimal performance over the long term (see Figure 5). RL is commonly used in domains requiring continuous decision-making, such as autonomous driving, game-playing optimization (e.g., Go and chess), robot control, financial trading, etc. Through interaction with the environment, agents gradually learn to devise optimal strategies to achieve their goals.

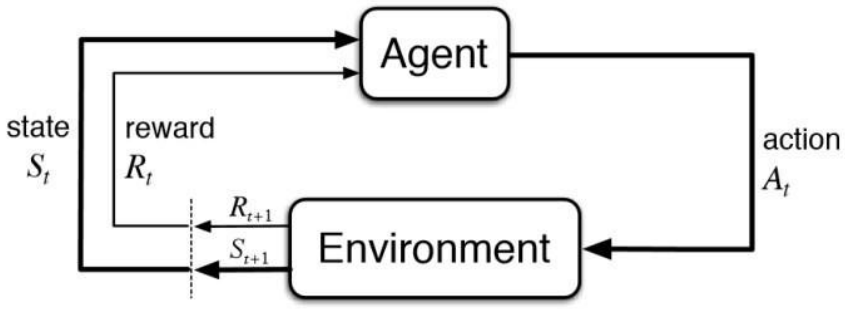

Figure 5. Principle of reinforcement learning.

2.2. Human Knowledge Engineering

Human knowledge engineering is one of the most important branches of artificial intelligence. It concerns how to collect, organize, represent, store, and apply human knowledge to enable computer systems to perform intelligent tasks [13]. Knowledge engineering aims to transform human experts' knowledge into forms that computers can understand and utilize. It includes expert systems, knowledge-based systems, knowledge bases, as well as knowledge bases, knowledge bases, inference and modeling methods, and related mathematical tools. In the engineering domain, knowledge engineering has extensive applications, helping engineering projects to be planned, designed, executed, and maintained more efficiently and reliably. Utilizing knowledge engineering techniques to build expert systems, these

systems can simulate domain experts' knowledge and decision-making processes. Constructing knowledge bases and ontologies in engineering is also crucial for storing and organizing domain knowledge. These knowledge bases can include design specifications, best practices, case libraries, etc. Knowledge engineering faces challenges such as difficulties in knowledge acquisition, complexity in knowledge representation, and issues in knowledge maintenance. With the development of big data and machine learning, knowledge engineering will continue evolving, supporting intelligent decision-making and autonomous systems. The most used concepts and methods in human engineering are described below.

(1) **Knowledge representation**: Knowledge representation is one of the most critical issues when developing expert and knowledge-based systems' cognitive architectures. It will enable simulation of human behaviors in understanding, reasoning, and interpreting knowledge to archive various human tasks. The tools for knowledge representation include:

- **Logical Representation:** representing knowledge in symbolic logic or rule-based systems, using formal language to express and infer new knowledge.
- **Semantic Networks:** representing knowledge through nodes and links, where nodes represent concepts or objects, and links represent relationships between them.
- **Frames:** representing knowledge in a structured form called frames, which capture the properties and attributes of objects or concepts and their relationships.
- **Ontologies:** representing knowledge in a formal, explicit specification of concepts, properties, and their relationships within a specific domain.
- **Neural Networks:** representing knowledge in the form of patterns or connections between nodes in a network, which can be used to learn from data and infer new knowledge.

(2) **Knowledge Base (KB):** A Knowledge Base is a collection of organized knowledge and information, typically existing in the form of a computer system, for retrieval, querying, and application as needed [14]. The knowledge base is part of knowledge management, aimed at capturing, storing, and organizing domain-specific knowledge to support decision-making, problem-solving, learning, and automation task execution. Knowledge bases contain organized and structured knowledge for easy retrieval and understanding by users. This typically includes concepts, relationships, rules, facts, descriptions, and explanatory information. KBs are usually oriented towards specific domains or topics, such as medicine, law, engineering, finance, etc. They are designed to provide accurate knowledge support within a specific domain. KBs are used not only for storing knowledge but also for retrieving and querying knowledge. Users can query the knowledge base to obtain the desired information and answers. KBs can be used for various purposes, including problem-solving, decision support, automation task execution, training, and learning. They can be integrated into various software applications to enhance their functionality. KBs typically require regular updates to reflect new knowledge, discoveries, and changes. This can be achieved through manual updates or automation. KBs can adopt different knowledge representation methods, including ontologies, rules, graphical models, databases, text documents, etc. The specific representation method depends on the design and application domain of the knowledge base. Based on the previous concepts, a knowledge-based system can be developed by combining three components: a human interface, a knowledge base and a knowledge inference engine (See Figure 6).

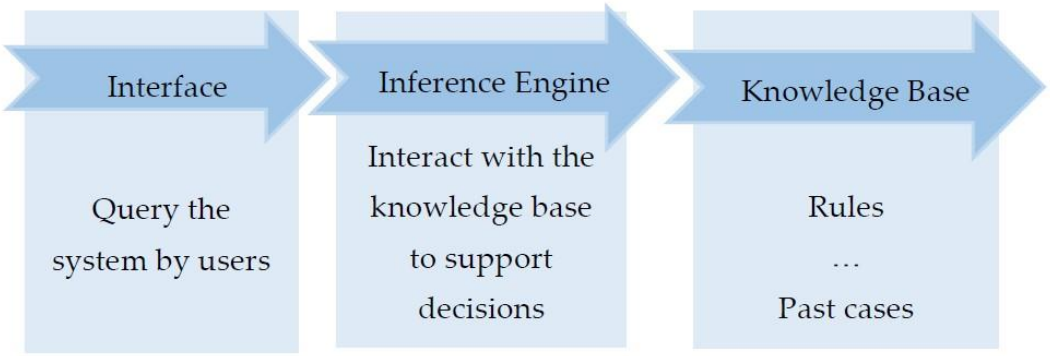

Figure 6. Knowledge-based systems architecture.

(3) **Experts Systems:** An expert system is a knowledge-based system that simulates human experts' thinking and decision-making process in a specific domain [15]. It also contains the three components of a knowledge-based

system and solves specific problems by using interactions of the inference engine and knowledge base and continuously updating the knowledge base with new data. There are three characteristics that every expert system should possess: (1) Consistency, which refers to the ability to obtain the same results from the same input set; (2) Availability, implying that the knowledge of the expert system is always present and is inherently built-in, without requiring years of training like human experts; (3) Comprehensiveness, which refers to the ability to gather knowledge from different human experts, thereby producing different relevant outputs. Finally, expert systems are seen not only as tools to assist human experts but also as substitutes for decision-making.

The mathematical tools and techniques for handling human knowledge, reasoning and inference mainly include the following aspects:

- **Logical Reasoning:** This includes first-order logic and predicate logic. First-order logic is used to represent and reason about complex knowledge about the world. It allows us to use predicates, variables, quantifiers, and logical operators to describe statements about objects and relationships, which is very useful in knowledge graphs and expert systems.
- **Graph Theory:** Graph theory represents and processes complex relationships and network structures, such as knowledge graphs and social networks [16]. Graph algorithms and traversal techniques help extract useful information from graph data.
- **Fuzzy Logic:** Fuzzy logic allows handling uncertainty and fuzziness, which is useful in fuzzy reasoning, control, and natural language processing [17].
- **Probabilistic Graphical Models:** Probabilistic graphical models such as Bayesian networks and Markov random fields are used to model uncertainty and inference. They have wide applications in knowledge representation and inference, especially in probabilistic knowledge inference.
- **Semantic Networks and Ontologies:** Semantic networks [18] are a graphical structure used to represent knowledge, while ontologies [19] are a formal framework for defining concepts and relationships. These methods are used in knowledge engineering and natural language processing to build shared knowledge bases.
- **Machine Learning:** Machine learning methods such as decision trees, support vector machines, neural networks, etc., can be used to learn patterns and regularities from large-scale data, for example, using collaborative filtering algorithms in recommendation systems to infer user interests.

2.3. Hybrid Modeling

A hybrid model is a gray box model, which is a model that lies between white box models (based on fully known theory or principles) and black box models (based on data and statistical methods, without considering specific internal mechanisms). The concept of a hybrid model originated in the field of neural networks. Its basic principle is to combine physical chemistry knowledge (also known as first-principle knowledge) with neural network models to establish hybrid models consistent with physical chemistry principles and measured data [20]. Compared to traditional physical chemistry models, hybrid models have better predictive accuracy, and better interpolation, extrapolation, and explanatory capabilities compared to models based on neural networks only. It balances the advantages and disadvantages of strict first-principle modeling and data-driven modelling.

The most important issue in hybrid modeling approaches is finding an appropriate combination mechanism for various models. There are three basic combination configurations, i.e., parallel and serial model structures. According to the description in [4], a hybrid model can adopt a parallel structure if (1) the parametric model (physical-chemical laws) can independently of the nonparametric model (data mining) describe the system's behavior and (2) the nonparametric model improves the prediction quality of the parametric model, aiming to obtain a good agreement with the real system. Moreover, a serial structure will enable the hybrid model to have interesting properties, namely a reduction in the data requirements, improvement in extrapolation performance, and improved systems understanding.

Hybrid modeling has numerous applications in chemistry, biology, and mechanical engineering. For example, in establishing chemical reactors and digital twins for metallurgical processes, fundamental chemical reaction laws and processes should be taken into account in the models. Common first-principle knowledge includes material and energy balances, thermodynamic laws and reaction kinetics, as well as certain empirical models describing diffusion, heat conduction, and gas behavior. In general, since these laws often describe macroscopic, general patterns of industrial processes under certain assumptions but do not accurately capture the microscopic, specific phenomena occurring in engineering, combining first-principle knowledge with data-driven models based on real-time measurement data can result in comprehensive models of different scales, from system macroscopic to microscopic details, and their related

digital twins. In hybrid models, commonly used data mining methods include ANNs, support vector regression (SVR), partial least squares (PLS), and various other methods.

Hybrid modeling plays a crucial role in material design by combining multiple modeling techniques to enhance accuracy, efficiency, and versatility in predicting material properties and behaviors. It contributes to material design in the following aspects:

- **Integration of Multiple Scales:** Hybrid modeling allows the integration of models at different scales, such as atomistic, mesoscale, and continuum, to capture the full range of material behavior accurately. It provides a more comprehensive understanding of material performance [21].
- **Combining Different Techniques:** Hybrid modeling combines diverse modeling techniques, such as molecular dynamics, finite element analysis, and machine learning, to leverage the strengths of each approach.
- **Optimization of the searching space:** By combining simulation and optimization techniques, researchers can efficiently search for materials with desired properties while considering various constraints and objectives.
- **Accelerating Material Discovery:** Hybrid modeling accelerates material discovery by reducing experimental tests. Virtual screening of materials using computational models can significantly narrow down the pool of candidates for further experimental validation, saving time and resources [22].

2.4. Multicriteria Optimization

Multicriteria optimization (MCO), also known as multi-objective optimization, refers to the process of optimizing a system, design, or decision with respect to multiple, often conflicting objectives or criteria. Its goal is to identify solutions representing a balance or trade-off between different objectives rather than optimizing for a single best solution. These objectives may include maximizing profit, minimizing costs, maximizing performance, minimizing risk, satisfying constraints, and achieving other desirable outcomes. The engineering applications of MCO mainly include the following two approaches:

(1) **Based on Solution Approach**: including

- **Mathematical Programming** methods such as goal programming, weighted sum method, lexicographic method, and constraint method;
- **Evolutionary Algorithms (EAs)**, such as genetic algorithms (GA), and evolutionary strategies (ES), which are metaheuristic optimization techniques inspired by natural evolution for exploring the solution space iteratively to find Pareto-optimal solutions [23];
- **Swarm Intelligence**, such as particle swarm optimization (PSO) and ant colony optimization (ACO), is inspired by the collective behavior of social insects or animals to search for Pareto-optimal solutions based on decentralized communication and cooperation among individuals.
- **Metaheuristic Methods**, such as Simulated Annealing, Tabu search, for iteratively improving candidate solutions without relying on gradient information.
- **Heuristic Approaches**, using rule-based or problem-specific strategies to explore the solution space efficiently.

(2) **Based on Decision Space Exploration:**

- **Exploratory Methods**, focusing on exploring the solution space to identify a diverse set of Pareto-optimal solutions by prioritizing solution diversity and coverage of the Pareto front.
- **Refinement Methods**: aiming to improve the quality of solutions found in the vicinity of the Pareto front. They often involve iterative improvement techniques to refine candidate solutions.
- **Interactive Methods**, involve human decision-makers in the optimization process, allowing them to provide feedback, adjust preferences, and steer the optimization toward desired regions of the Pareto front.

In the solution-based approach, evolutionary algorithms are the most used techniques in the optimization of engineering problems. A major advantage of EAs is that they are population-based metaheuristic methods. This is analogous to having an entire search party exploring the fitness landscape(s) on the lookout for the globally optimal solution(s), rather than a single person. As a result, large and rugged search spaces can be explored more effectively and efficiently because using a search party rather than a single person enables a greater area of the search space to be covered [24].

Decision space exploration involves systematically examining different combinations of decision variables to identify the optimal solution. In this scope, multicriteria decision-making has been widely used to evaluate a finite

number of predetermined alternatives, which are associated with a level of achievement of the criteria. Based on the criteria, the alternatives are selected or ranked. The concerned methods, including group decision-making models [25] and aggregation approaches [26], have been extensively studied in the literature. New Product Development (NPD) evaluation, including material design and discovery, is a dynamic decision with multiple criteria involving human cognition, technical standards, costs, environmental impacts and complex socio-economic factors [27]. A hierarchical model and computations for garment NPD comprehensive evaluation with multiple criteria have been given in [28]. These criteria have different roles and relevance to a design theme. For example, if the design theme is "well-being," i.e., to assess which garment product best matches the features of a well-being design and owns the well-being experience in wearing. This design theme needs to assess the criteria, which include factors related to garment function properties and fashion styles and marketing demands (See Figure 7).

In this evaluation model, numerical data taken from physical measures (e.g., surface friction, density) and linguistic data provided by human experts (e.g., pleasure, relaxation) are combined to jointly characterize the profile of a specific product design scheme. The weights of different criteria can also be qualitatively determined from pairwise comparisons of these criteria by experts according to their knowledge on the specific product and application. Therefore, the main issue of the multicriteria evaluation is to find an appropriate method based on the nature of the learning datasets to rank all possible design solutions and select the best one.

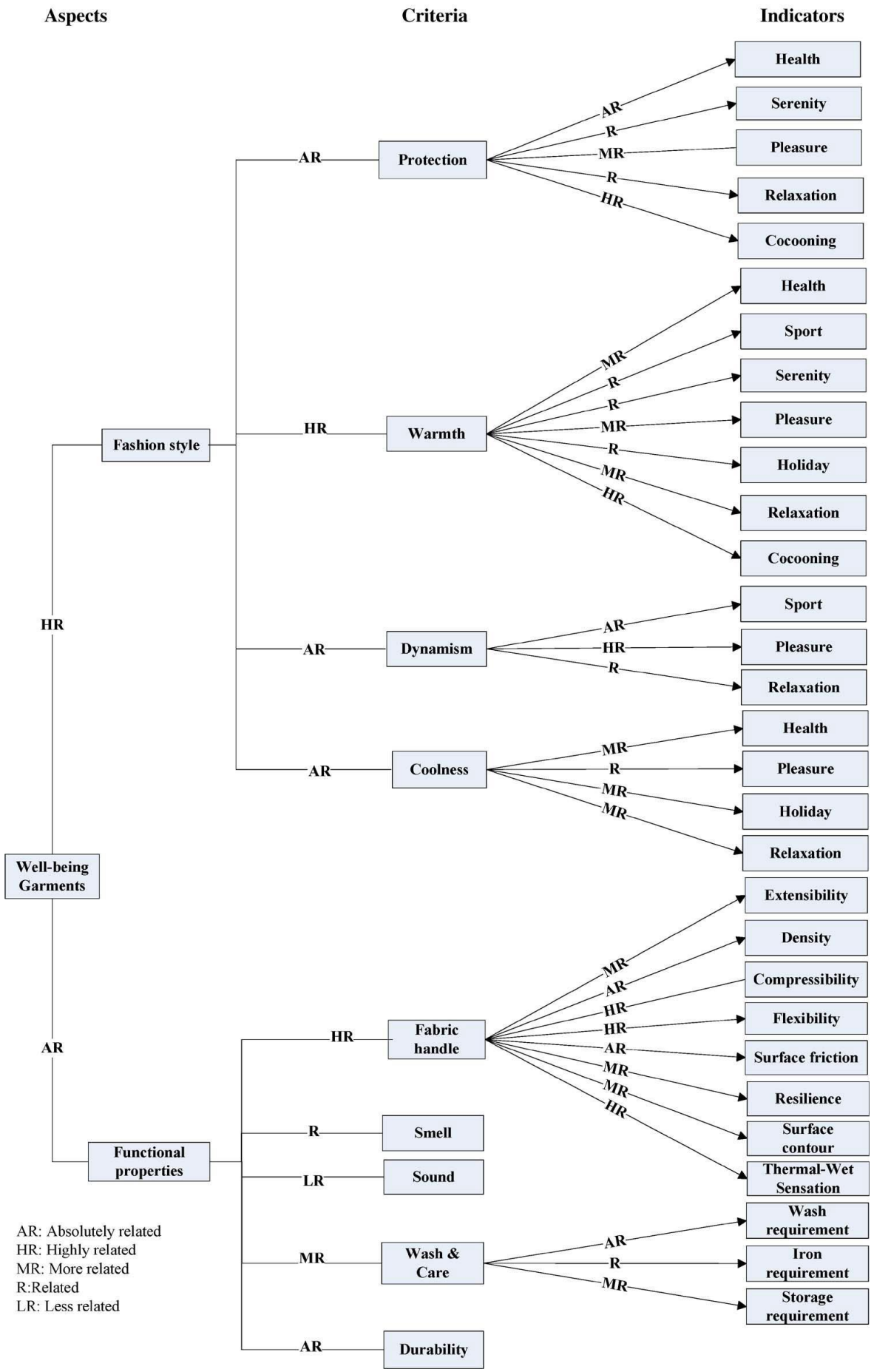

Figure 7. Hierarchical garment NPD evaluation model under the well-being theme (provided by [28]).

In multicriteria decision-making, one of the classical methods is to use decision priorities based on weights. However, soliciting weights (or priorities) from managers is a complex task, and calculating weights also requires selecting the best alternatives. The presence of qualitative variables further increases the complexity of this process. One method for multicriteria decision-making is the Analytic Hierarchy Process (**AHP**) developed by Saaty [29]. Decision-makers use AHP to decompose decision problems into relevant criteria and alternatives. AHP separates the analysis of criteria from alternatives, which helps decision-makers focus on the small, manageable parts of the problem. AHP handles qualitative and quantitative decision criteria in a relatively structured manner, allowing decision-makers to make balanced decisions quickly and "professionally."

TOPSIS (Technique for Order of Preference by similarity to Ideal solution) is another multicriteria decision-making method developed by Ching-Lai Hwang and Yoon [30]. TOPSIS was first proposed in a crisp version as a linear weighting technique, and after that, it is commonly used to solve the Multi-Criteria decision problems in various engineering and management fields. It works on the principle of geometric distance for selected alternatives; the shortest distance is the positive ideal solution, and the largest is the negative ideal solution [31]. Geometric distances are calculated and summed, and alternatives are chosen based on maximum similarity. Most of the time, experts find it difficult to allocate the score to the alternatives considered for the evaluation. Therefore, the fuzzy approach gained importance for fuzzy numbers over-allocating a precise score.

PROMETHEE (Preference Ranking Organization Method for Enrichment Evaluations) is a multicriteria decision-making technique based on construction of a partial pre-order [32]. It is based on an extension of the notion of criterion by introducing a function expressing the decision maker's preference for an action compared to another action. For each criterion, the decision maker is requested to choose one specific curve shape (e.g., linear, Gaussian). The parameters relating to each curve represent indifference and/or preference thresholds.

AHP, TOPSIS, and PROMETHEE are three classical structured multicriteria evaluation methods frequently used in management and engineering to rank alternatives and select the best one. By introducing AI techniques to these methods, the structures and parameters of these methods can be further improved for adaptation to different uncertain scenarios. Especially, fuzzy techniques are usually integrated into these methods in order to process uncertainty related to experts' evaluation results. The specificities of each method are described in Table 1.

Table 1. Comparison of the three multicriteria evaluation methods.

Criteria of Comparison	AHP	TOPSIS	PROMETHEE
Nature of Criteria and Alternatives	Suitable for situations where criteria and alternatives are hierarchically structured. Decomposition of complex problems into a hierarchy of criteria and sub-criteria.	Do not require a hierarchical structure for criteria and alternatives. Evaluate alternatives based on their similarity to the ideal solution and dissimilarity to the worst solution.	Applicable when criteria and alternatives are not necessarily hierarchically structured. Focus on pairwise comparisons between alternatives based on each criterion.
Preference Modeling	Use pairwise comparisons to derive preference weights for criteria and alternatives. Require decision-makers to assess the relative importance of criteria and the performance of alternatives with respect to those criteria.	Calculate the relative closeness of each alternative to the ideal solution and the relative distance from the worst solution. Do not explicitly model preferences but focus on identifying the alternative that best balances proximity to the ideal solution and distance from the worst solution.	Employ preference functions to model the preference of one alternative over another for each criterion. These preference functions can take various forms, such as linear, Gaussian, or logistic functions.
Ranking and Decision Making	Provide a ranking of alternatives based on their overall weighted scores, considering both the importance of criteria and the performance of alternatives with respect to those criteria.	Rank alternatives based on their closeness to the ideal solution and distance from the worst solution. The alternative with the highest relative closeness is considered the most preferred.	Generate a partial ranking of alternatives based on pairwise comparisons for each criterion. These partial rankings are aggregated to obtain an overall ranking using various aggregation methods.
Sensitivity Analysis	Allow for sensitivity analysis to assess the robustness of results by examining the impact of changes in criteria weights.	Do not inherently include sensitivity analysis, but variations such as fuzzy TOPSIS allow for uncertainty analysis.	Perform sensitivity analysis to evaluate the stability of rankings with respect to changes in preference functions or criteria weights.

Moreover, a new trend is to combine the classical multicriteria optimization approaches with incremental learning. This combination can make decision-making processes dynamic by incorporating continuous learning and adaptation to new data. For example, dynamic criteria and alternative evaluation using fuzzy models and rough sets have been used

to deal with decision-making in a big data environment [33]. Also, Reinforcement learning has been used to adjust the AHP model based on the success or failure of previous decisions, leading to improved decision-making over time [34].

3. AI-Based Modeling and Prediction for Material Design

Currently, a large number of works on AI-based material design deal with modelling and prediction of materials compositions, structures (e.g., porous structure, surface textures, microstructures) and functional properties (e.g., heat and water flow dynamics) as well as relevant feature selection/extraction by learning from experimental data. The AI techniques can effectively support designers in finding relevant materials composition for a given functional property or product performance and, discover new materials with expected features, and preventing structural changes in the wrong direction. Most of these works (about 81% of papers on AI-based material design indexed in ScienceDirect) adopted various models of neural networks (including CNNs). These works are generally based on the existing ANN models (e.g., MLP, SVM, CNN) mentioned previously in Section 2. However, some special ANN models (e.g., physics-informed neural network (PINN) [35] and meta-surface ONN [36]) have been developed for the adaption of prediction models to various physical environments.

Moreover, computer vision techniques are usually used to extract information on material surfaces and structures from images or videos, which are considered non-destructive testing methods. For example, AI techniques (e.g., SVM, CNN) have been combined with image analysis (filtering, classification) to realize Structural Health Monitoring for quality control, flaw detection and performance prediction in advanced concrete materials [37]. The combination of material, visual data and physically measured data enables to enhance designer's understanding of materials further and improves the prediction capacity of ANN models. Several representative AI-based material design cases are described below, dealing with material structure design, meta-surface design, thermal flow prediction, and porous composite design.

An artificial intelligence-aided design strategy has been proposed in [38] for controlling lattice structures to obtain results close to the target anisotropy properties. This study is composed of two main steps. First, several 3D-CNN neural networks are used to predict the mechanical properties of filled lattice structure models. Second, several genetic algorithms are used to control the subunits of the lattice meta-structures in order to fill these lattice structures and intelligently design different anisotropies. The proposed 3D CNN models will replace the homogenization computation process, which is time-consuming. This treatment will enable the quick prediction of equivalent mechanical properties of lattice structures with any geometrical and material parameters. Next, the mesoscale design domain is divided into several subunits according to the encoded metaplot. At the last stage, a genetic algorithm is used to automatically adjust the combination type of the lattice structures for the involved subunits according to the predefined target anisotropic properties.

Recently, deep learning methods, i.e., graph-neural networks (GNNs), generative adversarial networks (GANs) and variational autoencoders (VAEs), have also been used to model material structures [39]. Especially, GANs enable the generation of realistic new material structures by setting up generative models based on random noises [40] due to their capacities to overcome the limitations of small experimental datasets, discover novel material compositions or structures and quickly training models for adaptation to various material properties. VAEs enable encoding and decoding materials structures into latent spaces to form generative models, leading to easier interpolation and manipulation [41].

The features of meta-surface miniaturization and its integration into advanced semiconductor processes have attracted numerous researchers. Traditional meta-surface design often requires experienced designers to master professional knowledge and skills. Therefore, design work has become rather difficult and time-consuming when the complexity of meta-surface design increases. The application of artificial intelligence in meta-surface design work has effectively reduced its development time and complexity. In this context, the meta-surface optical neural network (ONN) model has been constructed due to its high bandwidth, internal parallel computational mechanism, and high interconnectivity, enabling it to accelerate the efficiency of both software and electronic hardware [36]. The meta-surface ONN model can effectively code meta-surfaces based on dielectric material unit structures, which are hidden layers in optical neural networks.

The AI techniques are also used to model the thermal flow dynamics based on the Powell-Eyring non-Newtonian fluid law when the free stream condition is identical to stretching at the surface [42]. In this study, the temperature and concentration flow variables are considered simultaneously. Both injection and suction processes are realized at the surface. First, Partial Differential Equations (PDEs) are used to construct a mathematical model. The Lie symmetry Theory is used to develop a scaling group of transformations (SGT). Next, SGT is used to reduce the complexity of PDEs. The numerical solutions to these reduced PDEs can be obtained using shooting methodology. An ANN model is built to predict the skin friction coefficient (SFC) from the Powell-Eyring and suction parameters.

Another important issue in material design is accurately modeling and accurately modeling and predicting the fluid dynamics of water flow through porous media. For example, an accurate prediction of the speed of water flow inside the porous media will enable the computation of pressure drops. Computational fluid dynamics (CFD) are usually used to predict fluid dynamics. This classical method is efficient in terms of computational accuracy, but its computation load is rather heavy for more complex material geometries or fluid flow conditions. It has been revealed from practical cases that AI algorithms can realize the prediction of properties of fluid dynamics from physically measured data with reduced computational time and better prediction performance than classical computational laws. One example is provided in [43], in which computational fluid dynamics of water flow inside a pipe filled with copper porous media has been predicted by using the fuzzy bee algorithm (BAFIS), enabling the map of the generated CFD data to inlet velocities of several predefined flows.

The most important feature of porous composites is their special and diverse geometries related to material distribution, providing unique freedom in the design and optimization of structures. The morphology of internal pores is strongly related to special mechanical, chemical, biological, and electronic properties, making this new material/structural form appealing. There are two major categories of AI-based studies for mechanical analysis on functionally graded porous structures [44]. A straightforward means is to model relations between the material design parameters (lattice, honeycomb, and foam mesoscopic details) and the mechanical behaviors using machine learning techniques, enabling threduction of complex conventional computations based on physical laws. One example is provided by Chen et al. [45], who first adopted conventional neural networks to recognize the 2D RVE images of metal foams and the corresponding compressive stiffnesses and then realized an uncertainty analysis on the bending of functionality graded porous beams considering the prediction error rate of neural networks. Another research orientation is to simplify the solving of partial differential equations as governing equations of mechanical properties (bending, buckling, and vibration) with the aid of data mining algorithms without processing the porosity details. In this context, Bazmara et al. [35] proposed a physics-informed neural network (PINN) in order to predict the nonlinear bending responses of 3D FG porous beams. They highlighted that this model is much better than the classical finite difference method in terms of rapidity.

Uncertainty, usually occurring in material structures, can be modelled and analyzed using fuzzy techniques and combinations of fuzzy logic and neural networks. One example is the design of textile-reinforced concrete structures under the conditions of non-traditional uncertainties [46]. This study utilizes a finite element to model folded-plate structures. This so-called multi-reference-plane model (MRM) can effectively characterize the structure's performance strengthened by textile-reinforced concrete (TRC) layers using multi-Kirchhoff kinematics. Both experimental and numerical simulation results demonstrate that TRC's structural responses strongly depend on the spatial and temporal variation of uncertain material and geometry. For this purpose, this study focuses on modeling the generalized uncertainty caused by material and geometric parameters by using fuzzy techniques. The uncertainty models and the MRM are combined to form a fuzzy stochastic finite element model. In another study [47], an adaptive fuzzy neural network has been used to extract fuzzy rules directly from experimental data and model material properties. This model enables the prediction of material strength based on material compositions and its geometric microstructure. Compared with the results obtained by classical methods such as multiple statistical analysis, fuzzy regression and neural networks, the fuzzy neural network shows good performances in learning accuracy, generalization and interpretation.

One important trend in AI-based material design is to combine various AI tools in order to promote the materials discovery cycle by integrating data-driven modeling, simulation, and optimization techniques. For example, a study combining several AI tools has been proposed in [39] to address two key challenges in the design of ceramic electrochemical cells: (1) identifying the optimal doping level and stoichiometric or mixing ratio leading to maximizing the materials' conductivity, compatibility, stability and catalytic activity, and (2) reducing negative side effects such as phase segregation or degradation caused by infiltration, doping, mixing and exsolution. In this study, AI has been used to predict the optimal composition for a given property or performance target by exploring various combinations of elements or compounds, creating new and superior materials with better performances for the electrolyte and electrode materials. In general, ANNs and other data mining approaches can effectively address these two challenges by predicting the optimal material composition for a given property and discovering new materials with expected performance features. Moreover, maintaining the material structural stability and compatibility is another challenge in material design. One solution to address this challenge is to manipulate the materials' crystallographic arrangement and defect configuration to tune their transport and catalytic properties. In this situation, ANNs and other data mining approaches can be used to model the defect chemistry and thermodynamics of the materials and design new structures with improved performance features and stability. Finally, optimization of the material microstructural parameters is also a challenge that requires integration of the morphology, porosity, grain size, and grain boundary to enhance their

transport and reaction properties while maintaining their mechanical integrity and durability in thermal and electrochemical stress conditions. However, this challenge also gives an opportunity to create new and effective microstructures with improved properties by optimally combining the shape, size, orientation, and distribution of the grains and pores. This opportunity can be realized by using AI to simulate the material manufacturing and sintering processes and by optimizing the microstructure parameters for given material properties or functionalities.

4. Multicriteria Optimization

Multicriteria optimization techniques, including problem-based optimization approach and decision space exploration-based approach, mentioned in Section 2, are playing a crucial role in material design due to several important reasons:

(1) **Balancing Conflicting Objectives:** Material design often involves optimizing multiple conflicting objectives or criteria. For example, a material may need to possess high strength, durability, and low cost simultaneously. Multicriteria optimization techniques enable researchers to find trade-offs and compromises between these conflicting objectives, allowing for the development of materials that meet diverse requirements.

(2) **Enhancing Performance:** Multicriteria optimization enables the design of materials with enhanced performance across multiple dimensions. By considering various criteria such as mechanical properties, thermal conductivity, electrical conductivity, and environmental impact simultaneously, researchers can identify material compositions and structures that offer superior overall performance compared to single-criterion optimization approaches.

(3) **Tailoring Material Properties:** Multicriteria optimization facilitates the customization of material properties to suit specific applications or requirements. By considering multiple criteria, designers can fine-tune material compositions, microstructures, and processing parameters to achieve desired combinations of properties, enabling the development of materials with tailored functionalities for diverse applications.

(4) **Optimizing Across Multiple Scales:** Material design often involves optimization across multiple length scales, from atomic and molecular levels to macroscale properties. Multicriteria optimization techniques can integrate information from different scales and disciplines to design materials with optimized performance across the entire length scale spectrum, enabling the development of multiscale materials with superior properties and functionalities.

(5) **Accounting for Uncertainty and Variability:** Multicriteria optimization provides a framework for accounting for uncertainty and variability in material properties and performance. By considering multiple criteria and incorporating uncertainty quantification techniques, researchers can assess the robustness and reliability of material designs under different operating conditions and environmental factors, leading to more resilient and adaptable materials.

(6) **Promoting Sustainable Design:** Multicriteria optimization can help promote sustainable material design by considering both performance criteria and environmental, social, and economic factors. By incorporating sustainability metrics (such as Life Cycle Analysis indicators) into the optimization process, researchers can identify materials with reduced environmental impact, improved resource efficiency, and enhanced social acceptability, contributing to the development of more sustainable and eco-friendly materials.

The current studies dealing with multicriteria optimization are mostly based on evolutionary algorithms to find the most relevant technical parameters that meet the user's requirements on material functional and visual performances. There are also some studies on decision-making by selecting the most relevant alternatives from a finite set of candidates (design schemes or raw materials). Many works on material design combine different approaches (multicriteria optimization, modelling of relations between technical parameters and product performances, visual and functional simulations) in a complementary way in order to find the most relevant design solution. Several typical cases of multi-objective optimization for material design are described below.

Considering simultaneously multiple conflicting properties in alloy optimization design is necessary yet remains challenging. A strategy combining machine learning and multi-objective optimization based on thermodynamic simulation data was proposed to accelerate the composition design of Ni-based superalloys [48]. The material microscopic parameters were identified using Pearson correlation analysis and domain knowledge and then taken as the key factors affecting tensile strength and elongation. The Multi-Objectives Evolutionary Algorithm (MOEA) was used to search for a well-built surrogate by learning meta-heuristically for the Pareto front of three objectives and its responding Pareto optimal solution set of composition. Next, nine high-performance superalloy samples selected from the obtained Pareto front were fabricated and tested in the laboratory. A new composition among the nine tested samples was taken as the best one according to three pre-defined desired values of the following design criteria: the solvus temperature, volume fraction, and TCP phase content. This strategy, based on the cooperation of machine learning and

MOEA extends the methodology for multi-composition and multi-property design materials, which can simultaneously optimize multiple conflicting objectives rather than do one by one.

Ducobu et al. [49] give a study on the identification of input parameters of finite element model of the cutting process, i.e., material constitutive and friction models parameters, by integrating an Efficient Global Optimization (EGO) algorithm and an ALE orthogonal cutting model (Arbitrary Lagrangian-Eulerian formulations: solving partial differential equations (PDEs) that characterize the performance of materials under various conditions of solid mechanics and structural analysis.) into Coupled Eulerian-Lagrangian (CEL) formulations. The parameters identified by applying the proposed EGO surrogate-guided optimization method to an ALE-Eulerian model at an uncut chip thickness of 0.1 mm have been introduced to a CEL model.

Multi-objective optimization has also been involved in multifunctional material design in order to satisfy complex customer requirements and specifications with a reduced and optimized design cycle. Deng et al. [50] proposed an optimization method for designing multifunctional textile materials using intelligent techniques to determine a relevant operation setting space, which can help designers quickly realize a set of representative prototypesrealize a set of representative prototypes. In this approach, an appropriate online method for designing experiments has been developed to help designers recursively estimate the most appropriate values of design factors with a very small number of trials. In this online design of experiments, the values of design factors for new trials are determined according to the results obtained in previous trials. The proposed design support system enables combining experimental data and human knowledge on material design by using fuzzy rules techniques. The weights of quality restrictions and the thresholds for the degree of product acceptability and the reward probability are generated based on the professional knowledge of product/material experts and process operators.

Simonetti et al. [51] applied evolutionary optimization techniques to a specific multi-objective optimization problem, i.e., minimization of the Von Mises maximum stress and minimization of the maximum growth of the structure's internal strain energy. The global weighting method and the global criterion method have been proposed to achieve both the minimization of the maximum stress and the strain energy for optimizing the topology of two-dimensional elastic structures. Genetic algorithms have been used to remove inefficient materials and regions where the magnitude of stress or strain energy is relatively limited.

In Nagamadhu et al. [52], an approach of Multiple Criteria Decision Optimization helped to select the best material composites by evaluating the Ghatti gum reinforced with epoxy at various percentages with the multiple criteria of impact, tensile, hardness, and flexural properties. The weights for these mechanical properties have been assigned according to the Criteria Importance Through Inter-Criteria Correlation (CRITIC). The Entropy Method, Preference Selection Index (PSI), Multi-objective Optimization using the Basis of Ratio Analysis (MOORA), COMbinative Distance-based ASsessment (COMDAS), VIekriterijumsko KOmpromisno Rangiranje (VIKOR), Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) methods have been used to analyze the materials selection, optimize and grade combination of Ghatti gum weight fraction, leading to the best mechanical properties. From this approach, it has been found that 10% gum Ghatti exhibited the best mechanical properties.

Heat transfer augmentationusing nanomaterial particles in the base fluid has gained great attention in recent years. In this context, the design parameters for reaching the optimum performance of alumina nanomaterial particles and turbulence promotors in heat exchangers have been selected [53]. In this study, the AHP-TOPSIS technique has been applied to determine the optimal performance parameters in a heat exchanger and identify the best feasible option with simultaneous consideration of all the performance parameters dealing with friction as well as thermal features of a circular tube, i.e., length of twist, width of twisted tape; diameter protrusion, height of protrusion and nanoparticle concentration.

5. Hybrid Modeling Approaches

The use of hybrid modelling approaches, especially those combing physical-chemical computational laws and data mining-based models, has become an important trend in various scenarios of AI-based material design. The combination of data mining-based modeling, multicriteria optimization, and performance simulation has already been described in Section 4 and Section 5. Several cases of a combination of various models are described below.

In the design of advanced ceramic electrochemical cells, data mining approaches have been combined with the classical computational methods, such as density functional theory (DFT), molecular dynamics (MD), and finite element method (FEM), to develop hybrid models that leverage the strengths of both approaches [39]. In practice, data mining approaches can generate reduced-order models or surrogate models that can approximate the solutions of FEM simulations.

Parhi et al. [54] optimized the critical parameters of self-compacting geopolymer concrete (SCGC) with the objective to maximize compressive strength. This optimization process is very important for sustainable development. In this approach, a large representative database was carefully constructed by integrating data from various publications, with Fly ash and GGBFS serving as essential binders. Before the development of the machine learning model, a preprocessing process was implemented to ensure data quality. In order to optimize the overall material performances, three machine learning base models (AdaBoost, Random Forest Regressor, XGBoost) were adopted and their hyperparameters were diligently fine-tuned by using effective spotted hyena metaheuristic optimization technique. A hybrid model and a meta-learner were developed based on these three base models. This hybrid model outperformed other models due to its superior accuracy and generalizability. The hyperparameters of the hybrid model were further fine-tuned using metaheuristic methods to maximize its performance. This hybrid modeling process uses the strengths of individual models, i.e., three base models (AdaBoost, RFR, and XGBoost) by combining them in a complementary way to create a robust and accurate overall predictive model. The Extreme Learning Machine techniques were used to enhance the overall prediction performance.

Sustainability has been widely recognized as an added value in all engineering areas, including material design. A sustainable material design must consider both performance criteria and environmental, social, and economic factors in environmental research. Especially, CCUS (Carbon Capture, Utilization, and Sequestration) for decarbonizing energy and industries is a relevant measure to reduce the greenhouse effect. In this context, the AI-based design approaches usually combine modeling with multiple sources, multicriteria optimization, and simulation simultaneously. Al-Sakkari et al. [55] proposed a study for identifying the need for robust hybrid evaluation tools for CCUS modeling, simulation, and optimization based on the combination of artificial intelligence and related mechanisms (e.g., physical and chemical laws). sThus, the involved computational technologies for CCUS must enable the model related processes for CCUS, while evaluating the need for improvements or new developments to reduce the overall costs of CCUS system design and operations. In this study, the used techniques include first principles (physical laws)-based models for characterizing mass/energy conservation and equilibrium/thermodynamic relations (e.g., 3D computational fluid dynamics) and data mining-based models with different methods (ANNs, SVMs, decision trees, Random Forest, …) for the same relations. In the first-principles-based modelling, the complex multi-physics systems are modelled using commercial and robust software such as COMSOL and ANSYS. Besides, this paper also introduces a method of life cycle assessment (LCA) to evaluate CCUS systems, in which a combination of LCA and AI approaches is used. Other advanced methods using AI capabilities can be developed to optimize the whole CCUS value chain. This hybrid modeling approach can effectively accelerate the selection of optimal materials by providing relevant rules which accelerate the design of capture/utilization plants. Moreover, deep reinforcement learning coupled with process simulations will further improve process design/operations by simultaneously optimizing equipment sizing and operating conditions, and generative deep learning can be used as a key solution to optimize capture/utilization materials design/discovery.

6. Conclusions

This paper gives a comprehensive review of the applications of various AI techniques to advanced material design. Concretely, the basic concepts and fundamental methods frequently used in AI-based material design, as well as their representative real cases, have been systematically presented, providing a guideline to researchers in material design and development. The main application cases are diversified, covering not only control and optimization of multiscale structures (e.g., porous structures) in materials and their functional properties (e.g., heat flow and water flow) but also sustainable material design comprehensively taking into account multiple criteria (e.g., functional properties, costs, environmental impacts) in a balanced way. The research theme of AI-based material design is developing in breadth and depth. It is not limited to the optimization of a single design operation with data mining only but has a strong trend to hybrid modelling approaches by combining relevant AI techniques and classical physical and chemical laws as well as dynamic simulation of material functional and aesthetic performances in its various stages of implementation and use. Integrating various AI techniques to support the whole design process instead of a single design stage will be interesting for material designers. For this purpose, we consider that a complete material design environment can be created, covering digital twins of designed materials, involving implementation processes and users. The interactions between the real and digital design environments can be optimized using AI decision support tools with online comparisons between the predicted and real material performances. In this situation, the material prediction models will be quickly adjusted according to new data extracted online from the real design environment.

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References

1. Artificial Intelligence for Materials Design. Available online: https://www.mpg.de/20096180/artificial-intelligence-in-material-design (accessed on 31 March 2023).
2. Papadimitriou I. AI methods in materials design, discovery and manufacturing: A review. *Comput. Mater. Sci.* **2024**, *235*, 112793.
3. Raabe D, Mianroodi JR, Neugebauer J. Accelerating the design of compositionally complex materials via physics-informed artificial intelligence. *Nat. Comput. Sci.* **2023**, *3*, 198–209.
4. Schweidtmann AM, Zhang D, Stosch Mv. A review and perspective on hybrid modeling methodologies. *Digit. Chem. Eng.* **2024**, *10*, 100136.
5. Russell SJ, Norvig P. *Artificial Intelligence: A Modern Approach*, 3rd ed.; Prentice Hall: Hoboken, NJ, USA, 2010.
6. Azencott CA. *Introduction au Machine Learning*, 2nd ed.; Dunod: Paris, France, 2022.
7. Breiman L. *Classification and Regression Trees*, Taylor & Francis: New York, NY, USA, 1984.
8. Breiman L. Random forests. *Mach. Learn.* **2001**, *45*, 5–32.
9. Haykin S. *Neural Networks-A Comprehensive Foundation*; Maxwell MacMillian Int.: New York, NY, USA, 1994.
10. Alzubaidi L, Zhang J, Humaidi AJ, Al-Dujaili A, Duan Y, Al-Shamma O, et al. Review of deep learning: concepts, CNN architectures, challenges, applications, future directions. *J. Big Data* **2021**, *8*, 53.
11. Principe JC, Miikkulainen R. Advances in Self-Organizing Maps. In Proceedings of the 7th International Workshop, WSOM 2009, St. Augustine, FL, USA, 8–10 June 2009.
12. Barto RS, Sutton AG. *Reinforcement Learning: An Introduction*; MIT Press: Cambridge, MA, USA, 1998.
13. Brachman RJ, Levesque HJ. *Knowledge Representation and Reasoning*; Elsevier: San Francisco, CA, USA, 2004.
14. Ahmed A, Al-Masri N, Abu Sultan YS, Akkila AN, Almasri A, Mahmoud AY, et al. Knowledge-based systems survey. *Int. J. Acad. Eng. Res.* **2019**, *3*, 1–22.
15. Saibene A, Assale M, Giltri M. Expert systems: Definitions, advantages and issues in medical field applications. *Expert Syst. Appl.* **2021**, *177*, 114900.
16. Jia Y, Qi Y, Shang H, Jiang R, Li A. A practical approach to constructing a knowledge graph for cybersecurity. *Engineering* **2018**, *4*, 53–60.
17. Rajabi M, Hossani S, Dehghani F. A literature review on current approaches and applications of fuzzy expert systems. arXiv preprint arXiv:1909.0879. 2019. Available online: https://ar5iv.labs.arxiv.org/html/1909.08794 (accessed on 29 May 2024).
18. Berners-Lee T, Hendlert J, Lassila O. The semantic web. *Sci. Am.* **2001**, *284*, 5.
19. Hoang HH, Jung JJ. An ontological framework for context-aware collaborative business process formulation. *Comput. Inform.* **2015**, *33*, 553–569.
20. Zendehboudi S, Rezaei N, Lohi A. Applications of hybrid models in chemical, petroleum, and energy systems: A systematic review. *Appl. Energy* **2018**, *228*, 2539–2566.
21. Zhou T, Gani R, Sundmacher K. Hybrid data-driven and mechanistic modeling approaches for multiscale material and process design. *Engineering* **2021**, *7*, 1231–1238.
22. Fang J, Xie M, He X, Zhang J, Hu J, Chen Y. Machine learning accelerates the materials discovery. *Mater. Today Commun.* **2022**, *33*, 104900.
23. Lozanoa M, García-Martínezb C. Hybrid metaheuristics with evolutionary algorithms specializing in intensification and diversification: Overview and progress report. *Comput. Oper. Res.* **2010**, *37*, 481–497.
24. Maier HR, Razavi S, Kapelan Z, Matott LS, Kasprzyk J, Tolson BA. Introductory overview: Optimization using evolutionary algorithms and other metaheuristics. *Environ. Model. Softw.* **2019**, *114*, 195–213.

25. Lu J, Zhang G, Ruan D, Wu F. *Multi-Objective Group Decision Making: Methods, Software and Applications with Fuzzy Set Technology*; Imperial College Press: London, UK, 2007.
26. Liberatore JM, Stylianou CM. Expert support systems for new product development decision making: A modeling framework and applications. *Manag. Sci.* **1995**, *41*, 1296–1316.
27. Belliveau P, Griffin A, Somermeyer S. *PDMA ToolBook 2 for New Product Development*; Wiley: New York, NY, USA, 2004.
28. Lu J, Ma J, Zhang G, Zhu Y, Zeng X, Koehl L. Well-being theme-based evaluation in new product development using fuzzy hierarchical criteria group decision method. *IEEE Trans. Ind. Electron.* **2011**, *58*, 2236–2246.
29. Saaty TL. *Decision Making for Leaders, Vol. II*; RWS: Pittsburgh, PA, USA, 1996.
30. Hwang CL, Yoon K. *Multiple Attribute Decision Making: Methods and Applications*; Springer-Verlag: New York, NY, USA, 1981.
31. Chaghooshi AJ, Fathi RM, Kashef M. Integration of fuzzy Shannon's Entropy with Fuzzy TOPSIS for industrial robotic system selection. *J. Ind. Eng. Manag.* **2012**, *15*, 102–114.
32. Roy B. *Méthodologie Multicritère d'Aide à la Décision*; Economica: Paris, France, 1985.
33. Yang Y, Jie MQ, Chen ZS. Dynamic three-way multi-criteria decision making with basic uncertain linguistic information: A case study in product ranking. *Appl. Soft Comput. J.* **2024**, *152*, 111228.
34. Chen M, Xie Z, Sun Y, Zheng S. The predictive management in campus heating system based on deep reinforcement learning and probabilistic heat demands forecasting. *Appl. Energy* **2023**, *350*, 121710.
35. Bazmara M, Silani M, Mianroodi M. Physics-informed neural networks for nonlinear bending of 3D functionally graded beam. *Structures* **2023**, *49*, 152–162.
36. Lv J, Zhang R, Gu Q, Uddin MH, Jiang X, Qi J. Meta-surfaces and their intelligent advances. *Mater. Des*. **2024**, *237*, 112610.
37. Sarkar K, Shiuly A, Dhal KG. Revolutionizing concrete analysis: An in-depth survey of AI-powered insights with image-centric approaches on comprehensive quality control, advanced crack detection and concrete property exploration. *Constr. Build. Mater.* **2024**, *411*, 134212.
38. Ji Z, Li D, Liao W, Xie YM. AI-aided design of multiscale lattice meta-structures for controllable anisotropy. *Mater. Des.* **2022**, *223*, 111254.
39. Bello IT, Taiwo R, Esan OC, Adegoke AH, Ijaola AO, Li Z, et al. AI-enabled materials discovery for advanced ceramic electrochemical cells. *Energy AI* **2024**, *15*, 100317.
40. Guo K, Yang Z, Yu CH, Buehler M. Artificial intelligence and machine learning in design of mechanical materials. *Mater Horiz* **2021**, *8*, 1153–1172.
41. Lew AJ, Buehler MJ. Encoding and exploring latent design space of optimal material structures via a VAE-LSTM model. *Forces Mech.* **2021**, *5*, 100054.
42. Rehman KU, Shatanawi W, Malik MY. Group theoretic thermal analysis (GTTA) of Powell-Eyring fluid flow with Identical free stream (FS) and heated stretched porous (HSP) boundaries: AI Decisions. *Case Stud. Therm. Eng.* **2024**, *55*, 104101.
43. Alotaibi HF. Development of mechanistic-artificial intelligence model for simulation of numerical data of water flow in porous materials. *Eng. Appl. Artif. Intell.* **2023**, *126*, 106844.
44. Chen D, Gao K, Yang J, Zhang L. Functionally graded porous structures: Analyses, performances, and applications—A Review. *Thin-Walled Struct.* **2023**, *191*, 111046.
45. Chen D, Emami N, Rezaei S, Rosendahl PL, Xu BX, Schneider J, et al. AI enhanced finite element multiscale modelling and structural uncertainty analysis of a functionally graded porous beam. *Arxiv Prepr.* **2022**, arXiv:2211.01970.
46. Graf W, Hoffmann A, Möller B, Sickert JU, Steinigen F. Analysis of textile-reinforced concrete structures under consideration of non-traditional uncertainty models. *Eng. Struct.* **2007**, *29*, 3420–3431.
47. Hancheng Q, Bocai X, Shangzheng L, Fagen W. Fuzzy neural network modeling of material properties. *J. Mater. Process. Technol.* **2002**, *122*, 196–200.
48. Deng Y, Zhang Y, Gong X, Hu W, Wang Y, Liu Y, et al. An intelligent design for Ni-based superalloy based on machine learning and multi-objective optimization. *Mater. Des.* **2022**, *221*, 110935.
49. Ducobu F, Palanisamy NK, Arrazola PJ, Rivière-Lorphèvre E. Application of material constitutive and friction models parameters identified with AI and ALE to a CEL orthogonal cutting model. *Procedia CIRP* **2023**, *117*, 311–316.
50. Deng X, Zeng X, Vroman P, Koehl L. An intelligent multi-criteria optimization method for quick and market-oriented textile material design. *J. Glob. Optim.* **2010**, *51*, 227–244.
51. Simonetti HL, das Neves FA, Almeida VS. Multiobjective topology optimization with stress and strain energy criteria using the SESO method and a Multicriteria Tournament Decision. *Structures* **2021**, *30*, 188–197.
52. Nagamadhu M, Patil S, Kivade SB, Gunge A, Kadhim KF. Effect of Ghatti gum content on mechanical properties of epoxy composite using multicriteria optimization techniques. *Mater. Today Proc.* **2023**, *in press*, doi: 10.1016/j.matpr.2023.08.102
53. Kumar S, Maithani R, Kumar A. Optimal design parameter selection for performance of alumina nano-material particles and turbulence promotors in heat exchanger: an AHP-TOPSIS technique. *Mater. Today Proc.* **2021**, *43*, 3152–3155.
54. Parhi SK, Dwibedy S, Panigrahi SK. AI-driven critical parameter optimization of sustainable self-compacting geopolymer concrete. *J. Build. Eng.* **2024**, *86*, 108923.

55. Al-Sakkari EG, Ragab A, Dagdougui H, Boffito DC, Amazouz M. Carbon capture, utilization and sequestration systems design and operation optimization: Assessment and perspectives of artificial intelligence opportunities. *Sci. Total Environ.* **2024**, *917*, 170085.