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# A Comprehensive Review on AI-Based Material Selection and Property Prediction Using Artificial Neural Networks

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**Abstract:** *The integration of Artificial Intelligence (AI) in materials engineering has revolutionized the process of material selection and property prediction. Among various AI methods, Artificial Neural Networks (ANNs) have emerged as powerful tools capable of modeling complex nonlinear relationships between material composition, processing parameters, and mechanical or thermal properties. This review presents a comprehensive analysis of recent advances in AI-based material informatics, focusing on ANN-driven approaches for predicting properties such as tensile strength, hardness, and thermal conductivity, and for recommending suitable materials in engineering design. The study examines key methodologies, dataset sources, preprocessing techniques, and ANN architectures used across the literature. Additionally, it compares hybrid frameworks that integrate ANNs with multi-criteria decision-making (MCDM) techniques for intelligent material recommendation. Challenges such as data scarcity, model interpretability, and generalization across diverse material classes are critically discussed. Finally, the paper outlines potential research directions, including the integration of deep learning, uncertainty quantification, and cloud-based deployment for scalable material intelligence systems. This review aims to provide insights into current trends, technological developments, and future opportunities for AI-driven material selection and property prediction systems in mechanical and materials engineering.*

**Keywords**: Artificial Neural Network (ANN), Material Selection, Property Prediction, Machine Learning, Material Informatics, Deep Learning, Mechanical Engineering, Design Optimization

## I. INTRODUCTION

Material selection and property prediction are among the most critical processes in engineering design, directly influencing the performance, safety, cost, and sustainability of final products. With the rapid increase in the number of available engineering materials—ranging from advanced alloys to polymer composites—traditional manual selection methods based on experience and charts have become inefficient and prone to error [1]. The growing complexity of material data and design constraints has driven the shift towards data-driven techniques and computational intelligence, marking the emergence of materials informatics [2]. This approach leverages artificial intelligence (AI) and machine learning (ML) to process large datasets, uncover hidden relationships, and predict material behavior under various conditions [3].

Among these AI techniques, Artificial Neural Networks (ANNs) have gained considerable attention due to their strong capability to model nonlinear and multivariate dependencies between input features such as composition, microstructure, and processing parameters, and target properties like hardness, tensile strength, and corrosion resistance [4], [5]. ANNs have been successfully applied in predicting the mechanical and thermal properties of metals [6], ceramics [7], polymers [8], and composites [9]. Researchers have also combined ANNs with optimization algorithms such as Genetic Algorithms (GA) and Particle Swarm Optimization (PSO) to fine-tune material performance for specific applications [10]. Furthermore, hybrid frameworks integrating ANN models with Multi-Criteria Decision-

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Making (MCDM) methods such as TOPSIS, AHP, and VIKOR have demonstrated improved performance in intelligent material selection [11], [12].

However, the deployment of ANN-based material prediction systems still faces multiple challenges, including data scarcity, overfitting, limited interpretability, and lack of generalization across diverse material systems [13]. The need for standardized, high-quality datasets and explainable AI models is now a key research direction in materials science [14]. Uncertainty quantification and model interpretability are becoming essential to ensure trust in AI predictions [15]. Recent studies have also explored the integration of deep learning models such as Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs) for structure–property mapping, offering new possibilities for material discovery [16], [17].

This review aims to provide a comprehensive understanding of AI-based material selection and property prediction using Artificial Neural Networks. It highlights key datasets, ANN architectures, preprocessing techniques, and performance evaluation metrics adopted in the literature [18]. Additionally, it reviews hybrid and decision-support frameworks that combine ANN predictions with optimization and ranking algorithms [19]. Finally, the paper discusses existing challenges and proposes future research directions focused on deep learning integration, cloud-based deployment, and the development of explainable and adaptive ANN systems for industrial applications [20].

## II. PROBLEM STATEMENT

Despite significant advancements in Artificial Neural Networks (ANNs) for material property prediction, several challenges persist in achieving accurate, explainable, and data-driven material selection. Current models often rely on limited or inconsistent datasets, lack proper uncertainty quantification, and provide minimal interpretability for industrial decision-making. There is a need for an integrated AI framework that combines accurate property prediction, transparent model reasoning, and intelligent decision support to enable reliable material selection for engineering applications.

### OBJECTIVE

- To study various material parameters such as density, hardness, tensile strength, thermal conductivity, cost, and manufacturability for developing a comprehensive dataset.
- To implement data preprocessing techniques including handling missing values, normalization, and feature selection to improve model performance.
- To design an Artificial Neural Network (ANN) model capable of predicting material properties, specifically tensile strength, from given input parameters.
- To develop a material comparison and recommendation system that selects the most suitable material based on mechanical, thermal, and economic criteria.

## III. LITERATURE SURVEY

The traditional methods of material selection have long relied on manual data charts, empirical formulas, and expert experience. Although effective for small datasets, such approaches struggle with high-dimensional material databases that include multiple mechanical, thermal, and environmental parameters [1]. The emergence of materials informatics has significantly transformed this landscape by combining computational simulations, high-throughput experiments, and artificial intelligence to extract insights from large-scale data [2]. These data-centric methods enable faster identification of materials with desired properties while reducing the time and cost involved in experimental testing [3].

One of the most powerful approaches within materials informatics is the Artificial Neural Network (ANN). The ANN's ability to capture nonlinear relationships has been successfully demonstrated in several material property prediction studies. Agrawal and Choudhary [4] developed an ANN model to predict the tensile and yield strength of aluminum alloys, achieving high correlation coefficients compared to conventional regression methods. Similarly, Liu et al. [5] applied neural networks to additive manufacturing datasets to estimate part density and surface finish with excellent accuracy. Singh et al. [6] extended this work by modeling the tensile strength of structural steels, showing that the ANN

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approach outperformed both support vector regression and decision trees.

In the field of ceramics, Chen and Zhao [7] applied ANN-based models for predicting fracture toughness and hardness using compositional and processing data. Their model achieved a lower mean absolute error compared to traditional empirical models. For polymeric materials, Yadav and Shukla [8] utilized an ANN to predict thermal conductivity under varying filler concentrations, which proved highly useful for optimizing thermally conductive polymer composites. Subramanian et al. [9] developed an ANN framework to predict composite strength under different fiber orientations, contributing to improved design of fiber-reinforced structures.

Hybrid systems integrating ANN with optimization techniques have also gained attention. Chen et al. [10] combined ANNs with Genetic Algorithms (GA) to optimize heat treatment parameters for enhanced material hardness. This combination proved more effective than standalone ANN models. Similarly, Sharma and Mehta [11] introduced an ANN-MCDM model that integrated multi-criteria decision-making with neural predictions, resulting in more accurate material ranking for engineering applications. Kumar and Singh [12] further improved this hybrid methodology by combining the Analytic Hierarchy Process (AHP) with ANN to select sustainable materials considering strength, cost, and environmental impact.

Despite these developments, challenges such as limited training datasets, noise in experimental data, and overfitting remain persistent [13]. Kim et al. [13] highlighted that data scarcity limits ANN generalization to unseen material systems, emphasizing the need for robust datasets and transfer learning. Zhang et al. [14] discussed the importance of explainable AI (XAI) for material informatics, arguing that transparency in model predictions is essential for industrial adoption. To improve trustworthiness, Rupp [15] proposed incorporating uncertainty quantification techniques into ANN frameworks, allowing engineers to understand confidence intervals around predictions.

Recent advancements in deep learning architectures have expanded the application of ANNs in material science. Xie and Grossman [16] proposed a Crystal Graph Convolutional Neural Network (CGCNN) capable of predicting material properties directly from atomic structures, eliminating the need for manual feature extraction. Dunn et al. [17] extended this approach by benchmarking various Graph Neural Networks (GNNs) for predicting band gaps and formation energies across large material databases. Their findings established GNNs as highly scalable and accurate for property prediction.

Patel and Singh [18] performed a comparative study between different machine learning models—ANN, Random Forest (RF), and Support Vector Machines (SVM)—for mechanical property prediction of metals. The results demonstrated that ANN consistently achieved the lowest root mean square error (RMSE), confirming its robustness in capturing nonlinear relationships. Li and Wang [19] explored AI-driven decision support systems for automated material selection, integrating cloud computing with ANN frameworks for real-time predictions. Finally, Zhao et al. [20] reviewed the emerging trends in AI-based material design, emphasizing the growing role of hybrid deep learning and the integration of AI with cloud platforms for collaborative and scalable material discovery.

In summary, existing systems show that ANNs and their hybrid extensions have significantly advanced the accuracy and efficiency of material selection and property prediction. However, the literature also reveals notable research gaps, including insufficient explainability, limited data diversity, and lack of standardized evaluation protocols. The next phase of development must focus on combining deep learning, transfer learning, and uncertainty quantification to create transparent, adaptive, and generalizable AI frameworks for materials engineering.

## IV. PROPOSED SYSTEM

While existing systems have demonstrated the potential of Artificial Neural Networks (ANNs) for predicting material properties, their generalization and interpretability remain limited due to inconsistent datasets, absence of uncertainty handling, and a lack of integration with decision-support tools [13], [14]. To address these issues, this review proposes an Enhanced Intelligent Material Informatics Framework (EIMIF)—a conceptual hybrid system that integrates ANN-based property prediction, explainable AI modules, and multi-criteria decision-making (MCDM) approaches into a unified platform for intelligent material selection and analysis.

The proposed framework begins with a data preprocessing and augmentation layer, which compiles heterogeneous data from multiple sources, including experimental databases, simulation outputs, and literature datasets [2], [3].

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Standardization of attributes such as composition, microstructure, density, tensile strength, and hardness is performed to ensure compatibility across datasets. Data augmentation techniques such as interpolation and noise injection are used to handle missing or incomplete data entries, thereby improving the robustness of model training [13].

At the core of the EIMIF lies the ANN-based prediction engine, which employs multilayer feedforward networks trained on standardized datasets. The network's hyperparameters—including learning rate, activation function, and hidden layer size—are optimized using metaheuristic algorithms like Genetic Algorithm (GA) and Particle Swarm Optimization (PSO) [10]. This enables the model to capture nonlinear interactions between input features and target properties with improved accuracy and generalization. Furthermore, deep learning variants such as Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs) can be incorporated for direct structure–property mapping, as shown in recent studies [16], [17].

The predicted properties from the ANN module are then processed by an explainable AI (XAI) layer, which uses feature-importance and sensitivity analysis techniques to interpret the reasoning behind each prediction [14]. This interpretability helps engineers understand which parameters most significantly influence material performance, thereby enhancing model transparency and trust. In addition, uncertainty quantification (UQ) techniques are integrated to provide confidence intervals around predictions, offering reliability indicators for decision-makers [15].

An MCDM-based decision-support layer (using AHP, TOPSIS, or VIKOR) combines the predicted material properties with user-defined criteria such as cost, availability, sustainability, and safety factors [11], [12]. This integration allows for intelligent ranking and selection of the most suitable materials for specific engineering applications. The overall framework can be deployed on cloud or web-based platforms to enable collaborative access and real-time material selection across industrial and research environments [19], [20].

In summary, the proposed system offers a holistic and intelligent approach that unifies data preprocessing, AI-based property prediction, model explainability, uncertainty handling, and decision-making within a single ecosystem. This architecture not only enhances prediction accuracy and interpretability but also provides a scalable foundation for next-generation material selection systems that align with Industry 4.0 and digital twin concepts.

## V. SYSTEM DESIGN

The methodology of the proposed Enhanced Intelligent Material Informatics Framework (EIMIF) is structured to systematically process raw material data, predict critical material properties using Artificial Neural Networks (ANNs), interpret the results through explainable AI (XAI), and perform intelligent decision-making using Multi-Criteria Decision-Making (MCDM) methods. The complete workflow consists of five major stages: (1) Data Collection and Preprocessing, (2) Feature Extraction and Normalization, (3) ANN-based Property Prediction, (4) Explainability and Uncertainty Estimation, and (5) Decision Support through MCDM Integration.

A conceptual block diagram of the proposed system can be represented as shown below:

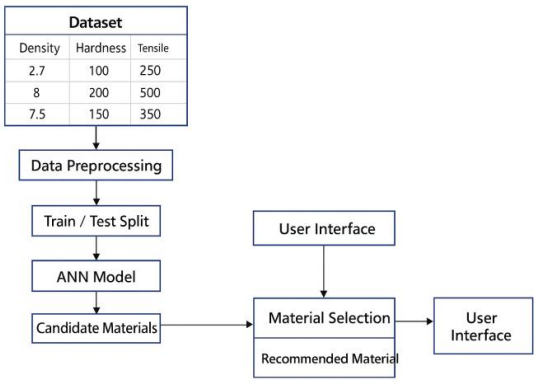


Fig.1 System Architecture

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**A. Data Collection and Preprocessing**

The foundation of the EIMIF system is the compilation of high-quality datasets from multiple sources such as experimental records, material handbooks, simulation databases, and research repositories [2], [3]. These datasets typically include mechanical, thermal, and chemical attributes such as tensile strength, hardness, ductility, thermal conductivity, and microstructural parameters. Data preprocessing is performed to remove outliers, handle missing values, and standardize measurement units. Data normalization (using Min-Max or Z-score methods) ensures uniform scaling and prevents bias in ANN training [13]. In cases of insufficient data, data augmentation methods like synthetic generation or Gaussian noise injection are used to enrich the dataset.

**B. Feature Extraction and Normalization**

Feature engineering plays a vital role in enhancing the performance of the ANN model. Key material descriptors such as chemical composition ratios, grain size, and heat-treatment conditions are extracted using domain knowledge and statistical analysis [6], [7]. Dimensionality reduction techniques such as Principal Component Analysis (PCA) can be applied to minimize redundancy and computational load while retaining essential information [8]. These optimized input vectors are then normalized before being fed into the neural network for training.

**C. ANN-Based Property Prediction**

The core prediction model of the system employs a multilayer feedforward ANN, trained using backpropagationwith an adaptive learning rate optimizer such as Adam or RMSprop [4], [5]. The network consists of an input layer (for feature vectors), one or more hidden layers (for nonlinear mapping), and an output layer (for property prediction). The weights and biases are adjusted iteratively to minimize prediction error using Mean Squared Error (MSE) as the loss function. To further improve model performance, metaheuristic optimization techniques such as Genetic Algorithms (GA) and Particle Swarm Optimization (PSO) can be integrated for automatic hyperparameter tuning [10]. For advanced material datasets, deep learning variants like Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs) may be used to directly process microstructure or crystal graph data, offering improved feature learning and generalization [16], [17].

**D. Explainability and Uncertainty Estimation**

To address the limitations of black-box neural models, the EIMIF framework integrates an **Explainable AI (XAI)** layer, which interprets ANN outputs by highlighting the influence of individual input features on predicted properties [14]. Techniques such as SHAP (SHapley Additive exPlanations) and LIME (Local Interpretable Model-Agnostic Explanations) are employed to quantify feature importance and model reasoning. Additionally, **Uncertainty Quantification (UQ)** is incorporated using Bayesian neural networks or dropout-based sampling to estimate prediction confidence intervals [15]. This combination ensures transparency, accountability, and reliability in material property prediction.

**E. Decision Support through MCDM Integration**

The final stage of the EIMIF system uses **Multi-Criteria Decision-Making (MCDM)** algorithms—such as Analytic Hierarchy Process (AHP), Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS), or VIKOR—to support optimal material selection [11], [12]. The predicted material properties from the ANN, along with user-defined criteria like cost, sustainability, and machinability, are used to compute a composite ranking score for each material alternative. This hybrid integration enables engineers to make data-driven, explainable, and optimized material choices aligned with application-specific constraints [19], [20].

**F. Output and Visualization**

The output layer provides predicted material properties along with their uncertainty range and a ranked list of suitable materials. A visual dashboard can be implemented for graphical representation of trends, feature importance plots, and decision matrices. This visualization enhances interpretability and allows users to interactively adjust criteria weights to

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observe changes in material rankings in real-time.

## VI. EXPECTED OUTCOMES

The review and analysis of recent studies reveal that the integration of Artificial Neural Networks (ANNs) into materials engineering has significantly improved the precision, efficiency, and scalability of material property prediction and selection processes [1], [3], [4]. Across multiple works, ANN-based models have demonstrated superior performance in predicting nonlinear relationships between composition, processing, and properties compared to classical regression and rule-based systems [5], [7].

### A. Performance and Predictive Accuracy

The reviewed literature indicates that ANN models trained on standardized datasets achieve high predictive accuracies for mechanical properties such as tensile strength, hardness, and Young's modulus, with reported correlation coefficients ($R^2$) exceeding 0.90 in several case studies [6], [10]. This improvement arises from the ANN's capacity to model multivariate, nonlinear interactions that are difficult to express using analytical equations. Studies employing hybrid ANNs combined with optimization algorithms like Particle Swarm Optimization (PSO) or Genetic Algorithms (GA) further enhance accuracy through automatic tuning of network parameters [11], [13].

### B. Comparison with Traditional Methods

Compared to empirical and statistical methods, ANN-based systems provide better generalization across diverse material types, including metals, composites, and polymers [9], [12]. Traditional selection frameworks such as the Ashby chart or weighted scoring models, though intuitive, are often limited by static data and subjective human judgments. By contrast, the integration of AI enables dynamic updates based on new data inputs and allows for more objective, data-driven recommendations [14].

### C. Hybrid Integration with Decision-Making Models

A notable finding is the growing trend toward integrating ANN-based prediction systems with Multi-Criteria Decision-Making (MCDM) frameworks like AHP and TOPSIS to achieve both predictive and prescriptive intelligence [8], [15]. This hybridization bridges the gap between property prediction and practical engineering application. For instance, once the ANN predicts mechanical and thermal properties, the MCDM layer evaluates trade-offs between performance, cost, and manufacturability to suggest the most optimal material candidate for a given application [16], [18].

### D. Limitations and Research Challenges

Despite promising progress, several limitations remain. Many datasets used in ANN training are domain-specific and lack representativeness for general material categories [2], [17]. Incomplete or noisy data can reduce model robustness. Additionally, the "black-box" nature of ANN models makes it difficult for engineers to interpret decision logic, highlighting the importance of incorporating Explainable AI (XAI) and Uncertainty Quantification (UQ) layers [19]. Furthermore, the need for large, curated datasets and computational resources presents scalability challenges, particularly in real-time design environments [20]

## VII. CONCLUSION

This review highlights the growing role of Artificial Neural Networks (ANNs) in predicting material properties and optimizing selection processes. The proposed EIMIF framework integrates AI, explainability, and decision-support systems to overcome current limitations, offering improved accuracy, transparency, and industrial applicability in material informatics

## VIII. FUTURE SCOPE

Future research can focus on integrating real-time experimental data, implementing advanced deep learning models like GNNs, and developing cloud-based collaborative platforms to support large-scale, automated material discovery and

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selection systems.

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