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Review paper

ISSN 0351-9465, E-ISSN 2466-2585

<https://doi.org/10.62638/ZasMat1837>



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(2026)

The evolving role of artificial intelligence in materials science: From data-driven discovery to future prospects

ABSTRACT

The incorporation of Artificial Intelligence (AI) into materials science has initiated a transformative shift, facilitating significant advancements in the discovery, optimization, and production of novel materials. This review provides a comprehensive overview of recent developments, uses, and problems that come with using AI in this area. It looks at cutting-edge methods like machine learning, neural networks, and genetic algorithms, and how they can help speed up the development of new materials. The main areas of use, such as finding new materials, improving the properties of existing ones, modelling and simulation, and improving manufacturing processes, are all discussed in depth. Even though a lot of progress has been made, there are still a lot of problems to solve, especially when it comes to data quality and availability, computational complexity, model interpretability, and ethics. This review includes case studies to show how AI-driven methods can be useful and effective in materials science. It also points out new trends and future directions, stressing the possibilities for collaboration between different fields and new research opportunities.

Keywords: Artificial intelligence, materials science, machine learning, optimization, innovation

1. INTRODUCTION

Artificial intelligence (AI) has influenced numerous areas of science and technology, such as materials science. The field of materials science is inherently complicated because there are so many different types of materials and their physical and chemical properties must be tailored to fit specific needs. In the past, finding and improving materials depended on trial and error and long, expensive experiments. But with the rise of AI, these processes have sped up and improved a lot [1-3].

Artificial Intelligence (AI), and more specifically, its most transformative subset, Machine Learning (ML), has made it easier than ever to process and analyze vast amounts of data. ML algorithms, such as deep neural networks, can identify complex patterns within datasets. This capability enables the optimization of material properties and the discovery of new, high-performing materials [2,4]. For instance, neural network models can leverage existing material databases to predict the properties of novel compounds, significantly reducing the reliance on costly and time-consuming experimental cycles [5-7].

The impact of Artificial Intelligence (AI) extends profoundly to materials modeling and simulation. By enhancing the accuracy of atomistic and molecular simulations, AI provides researchers with a powerful tool to forecast material behavior under diverse conditions [3,8,9]. This predictive capability is crucial for designing materials in demanding sectors such as aerospace, energy, and biomedicine, where performance and safety standards are exceptionally stringent.

AI is also important in materials science because it is used in manufacturing and production. AI algorithms can make manufacturing processes better, cut down on waste, and make the final products better. For example, AI-based control systems can change the settings for production in real time to keep quality high [10-13].

In short, adding AI to materials science has sped up the process of finding and improving materials and opened up new areas for research and new ideas. AI's ability to predict and analyze helps scientists solve problems that seemed impossible before and move materials science forward [1,3,12].

This review paper seeks to present a thorough examination of the advancements, practical implementations, and obstacles related to the utilization of artificial intelligence in materials science. To reach this goal, we concentrate on a few important areas.

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Paper received: 23.07.2026.

Paper corrected: 25.07.2026.

Paper accepted: 29.07.2026.

We will start by talking about the most recent progress in using AI techniques in materials science. This includes talking about machine learning techniques, neural networks, and other algorithms that are important to the process of finding new materials and improving the properties of materials that already exist [1-5].

Second, we will look at some specific ways that AI can be used in materials science. We will look at real-world examples of how AI has been used to find new materials, improve the properties of existing ones, model and simulate how materials behave, and make manufacturing and production processes better [6,7,10-14]. These examples will show how AI is changing different parts of materials science and how it can be useful in real life.

Third, we will discuss the problems and limits that come with using AI in materials science right now. This includes problems with the amount and quality of data that is available, the complexity of AI models and the need for computational power, as well as issues with how easy it is to understand and see through models. We will also talk about the moral and safety issues that come up as AI is used more and more [9,11,14].

Lastly, we will show some case studies that emphasize how AI can be applied in materials science. These case studies will show real-life examples of how AI has helped and what has been achieved, showing how it has affected research and industry in practical ways [10,12]. To sum up, we will talk about what the future holds and new trends in this field. We will emphasize research and innovation opportunities, along with the significance of interdisciplinary collaboration to address existing challenges and fully exploit the potential of AI in materials science [3,11]. Beyond a purely theoretical discussion, this review aims to demonstrate through concrete examples how these methodologies are implemented in practice and what tangible benefits they deliver. Detailed case studies such as the discovery of solid electrolytes through virtual screening (Section 7.1.1) and the real-time optimization of additive manufacturing

processes (Section 7.4.1) are woven throughout the analysis.

These examples are designed to give researchers and engineers a practical understanding of AI-driven workflows, the challenges involved in integrating them, and the scale of the progress they enable from improving specific material properties to dramatically accelerating development cycles.

This paper is for researchers, practitioners, and decision-makers who want to know more about how AI can be used in materials science. It seeks to provide comprehensive knowledge and insights to facilitate the continuous advancement and incorporation of AI into this dynamic and vital field.

2. STATE OF THE ART: AI APPLIED TO MATERIALS SCIENCE

Artificial intelligence (AI) has changed many areas of science, such as materials science. It has made a big difference in this field, especially when it comes to finding new materials, predicting how materials will behave, and improving manufacturing processes [3,15-17]. Recent advancements have concentrated on expediting the discovery and design of materials. In the past, these processes depended on experiments and simulations that took a long time and used a lot of resources. AI addresses these limitations by using algorithms to look at huge amounts of data, find patterns, and make very accurate predictions. For example, machine learning models have been used to predict the mechanical, electrical, and thermal properties of different materials. This means that fewer physical experiments are needed [5-7]. Another area of progress is improving the efficiency of material manufacturing processes. AI methods can optimize processing parameters, improve the quality of finished products, and reduce waste [11,13]. AI also plays a crucial role in modeling and simulation of material behavior in different situations. This helps us better understand and predict how materials will work in real-world situations [3,9,14].

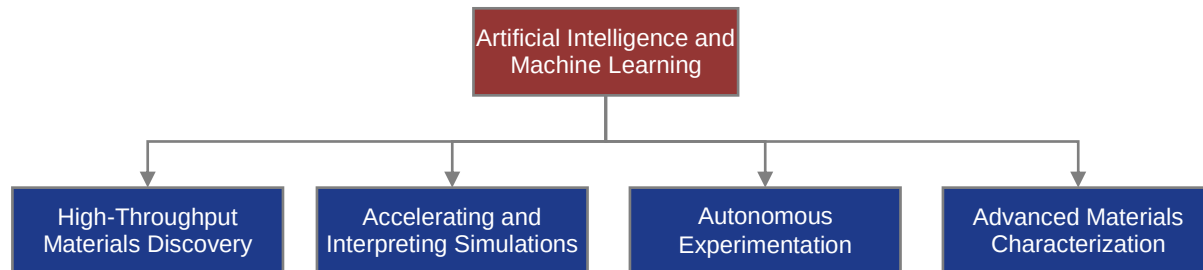


Figure 1. The main areas where AI and machine learning are used in materials science

Figure 1 shows a general view of the main areas where artificial intelligence (AI) and machine

learning (ML) are having a big effect on materials science. These methods are widely used to speed

up the discovery and design of new materials with specific properties, to identify useful structure-property relationships in large datasets, and to improve synthesis and processing conditions. Also, AI and ML techniques are being used more and more to look at microstructural images and spectral data. This lets computers automatically find and

sort features that would be impossible to achieve manually. These applications show how AI and ML are powerful tools for exploring the huge design space of materials. In the end, this will lead to a more efficient and predictive framework for materials research and development.

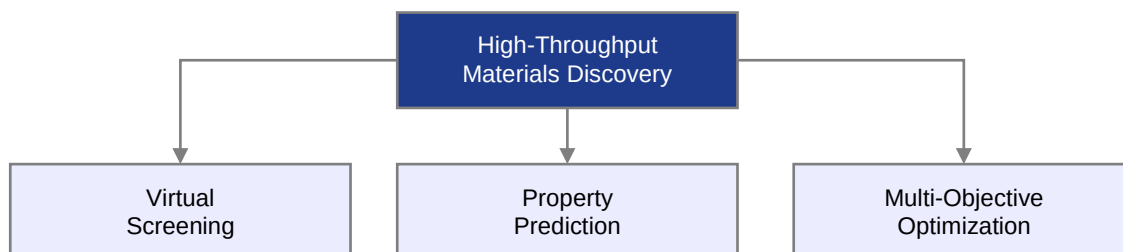


Figure 2. Important parts of designing materials for high-throughput

High-Throughput Materials Discovery is a new way of doing materials science that uses advanced computer and experimental methods to quickly find and improve new materials (Figure 2). Researchers can quickly look at thousands of potential materials in silico using virtual screening. This speeds up the initial discovery phase by putting the most promising candidates at the top of the list for further study. Property prediction models allow for the accurate determination of material properties like mechanical strength, thermal conductivity, or

electronic properties based on the material's composition and structure. This means that expensive and time-consuming experiments are less necessary. Also, multi-objective optimization techniques make it possible to optimize several material properties at once, which makes it easier to design materials with specific performance profiles for certain uses. This integrated approach cuts development times by a lot and makes materials innovation more efficient across a wide range of technological fields.

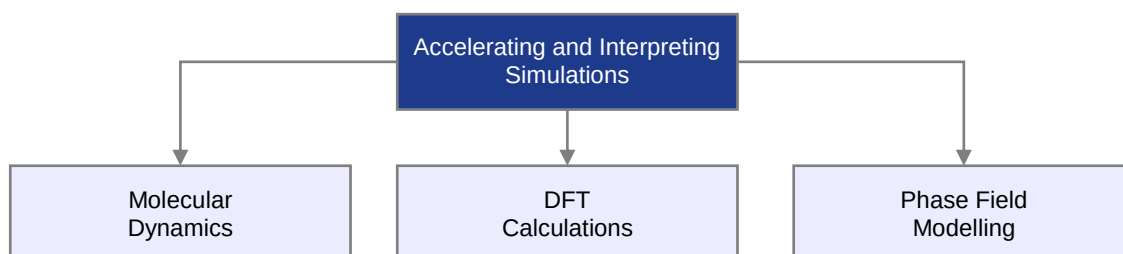


Figure 3. Machine Learning for Accelerating and Interpreting Computational Simulations

Accelerating and Interpreting Simulations has become a key part of modern computational materials science (Figure 3), where AI is changing the way models are made. In molecular dynamics, ML potentials and force fields make it possible to run simulations that last longer and cover bigger systems while still being accurate at the quantum level. This lets researchers study complex phenomena like defect migration and phase transformations that were too expensive to study before. For DFT calculations, machine learning interatomic potentials and surrogate models greatly lower the cost of electronic structure calculations. This makes it possible to quickly screen a lot of

materials across a wide range of chemical spaces. In phase field modelling, data-driven methods make it easier to set the parameters of free energy functionals and make better predictions about how microstructures change during the processing and synthesis of materials. These AI-enhanced simulation methods not only speed up computational workflows by a lot, but they also give us a better understanding of the physical world by using advanced pattern recognition and data interpretation tools. This closes the gap between atomistic simulations and how materials behave on a larger scale.

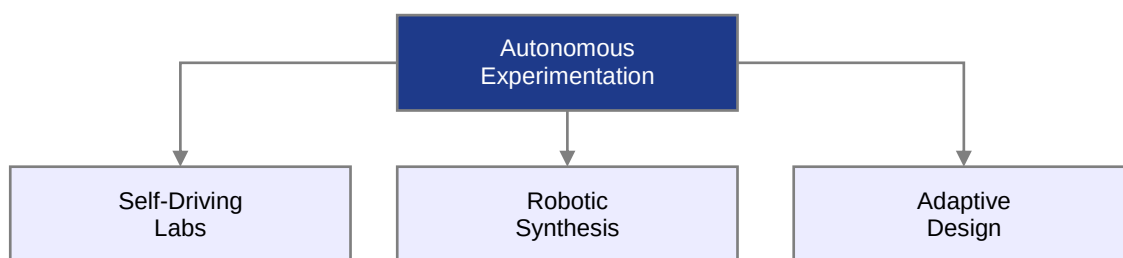


Figure 4. Key Parts of Independent Experimentation

Autonomous Experimentation is a new way of doing materials research that uses robotics, artificial intelligence, and advanced automation to change the way labs work (Figure 4). Self-driving labs use AI-based decision-making systems and automated synthesis platforms to plan, carry out, and analyze experiments with little help from people. They also learn from the results of experiments to improve research directions. Robotic synthesis allows for the rapid preparation of material samples with unmatched accuracy and repeatability. This makes it possible to quickly explore complicated parameter spaces like composition gradients, processing conditions, and synthesis protocols. Adaptive design systems use

Bayesian optimization and other machine learning algorithms to change experimental parameters on the fly based on real-time feedback. This helps them quickly find the best material formulations and processing conditions by exploring the multi-dimensional design space. This interconnected network of self-driving technologies speeds up the process of developing new materials from discovery to deployment. It also makes experiments more reliable and lets researchers explore parts of the materials space that were previously off-limits. This makes advanced materials research and innovation accessible to everyone.

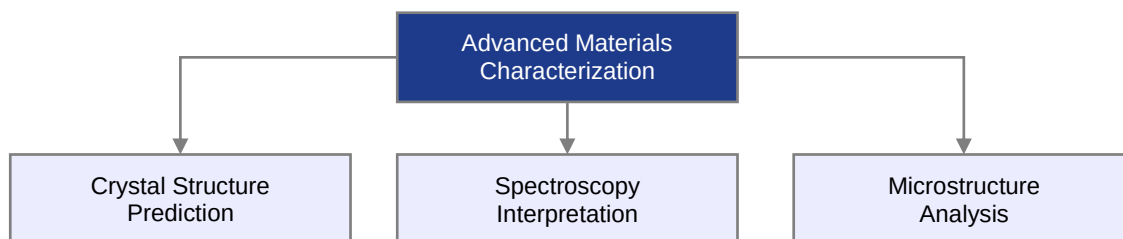


Figure 5. Sub-domains and particular applications of AI in materials science

Figure 5 represents the main sub-domains of Artificial Intelligence and their specific applications in materials science, including areas such as materials discovery, property prediction, microstructure analysis, and process optimization.

Artificial intelligence and machine learning have completely changed the field of advanced materials characterization, giving us never-before-seen information about how material structure and properties are related at different length scales. Deep learning algorithms that can quickly find stable polymorphs and guess unknown crystal structures from compositional information alone are helpful for predicting crystal structures. This speeds up the process of finding new materials with specific properties. Convolutional neural networks and pattern recognition techniques automatically analyze complex spectral data from techniques such as XRD, XPS, Raman, and NMR in spectroscopy interpretation. This makes it easy and quick to find chemical phases, bonding

environments, and functional groups that might be hard for human experts to find. Computer vision algorithms analyze large amounts of microscopy data from SEM and TEM images to 3D tomography to quantitatively describe features like grain boundaries, phase distributions, defects, and morphological patterns. This makes it possible to find statistical links between microstructural properties and how well a material works on a larger scale. These AI-enhanced characterization methods not only drastically reduce the time it takes for data analysis, but they also find hidden patterns and relationships in complex materials data. This helps scientists understand materials better and speeds up the creation of new materials for uses like energy storage and advanced manufacturing.

While these advancements paint a broad picture of AI's transformative role, their tangible impact is best understood through specific, quantifiable applications. The following sections will

delve into detailed case studies that exemplify this progress. For instance, the use of genetic algorithms to navigate complex compositional spaces (Section 7.1.2) and convolutional neural networks for real-time process control in additive manufacturing (Section 7.4.1) provide concrete evidence of how these theoretical frameworks are deployed to solve real-world materials challenges, yielding measurable improvements in properties, efficiency, and discovery rates.

3. ARTIFICIAL INTELLIGENCE TECHNIQUES

Artificial intelligence (AI) encompasses a wide range of computational techniques used to analyze complex data, generate predictions, and support optimal decision-making. Regression models, support vector machines, and ensemble methods are examples of machine learning algorithms that are often used to predict the properties of materials and sort structures. Convolutional and recurrent neural networks are two types of deep learning techniques that can pull high-level features out of images, sequences, and multidimensional datasets. To find the best material compositions and processing conditions, we use evolutionary

algorithms like genetic algorithms. These AI methods work together to make things more efficient, speed up discovery, and open up new possibilities in science and engineering.

The following are the most popular methods used in artificial intelligence (AI):

3.1. Learning Techniques:

Learning techniques, such as supervised [18], unsupervised [19], and reinforcement [20] learning, play a central role in analyzing and predicting material properties (See figure 6). For instance, supervised learning let us model complicated connections between input data and desired properties. Unsupervised learning, on the other hand, let us find patterns or groups in datasets that don't have labels [21,22]. Reinforcement learning, on the other hand, is increasingly leveraged to optimize manufacturing processes and material design [23]. When used with advanced algorithms like deep neural networks [24,25], these methods make it possible to make quick and accurate discoveries while lowering costs and time spent on development.

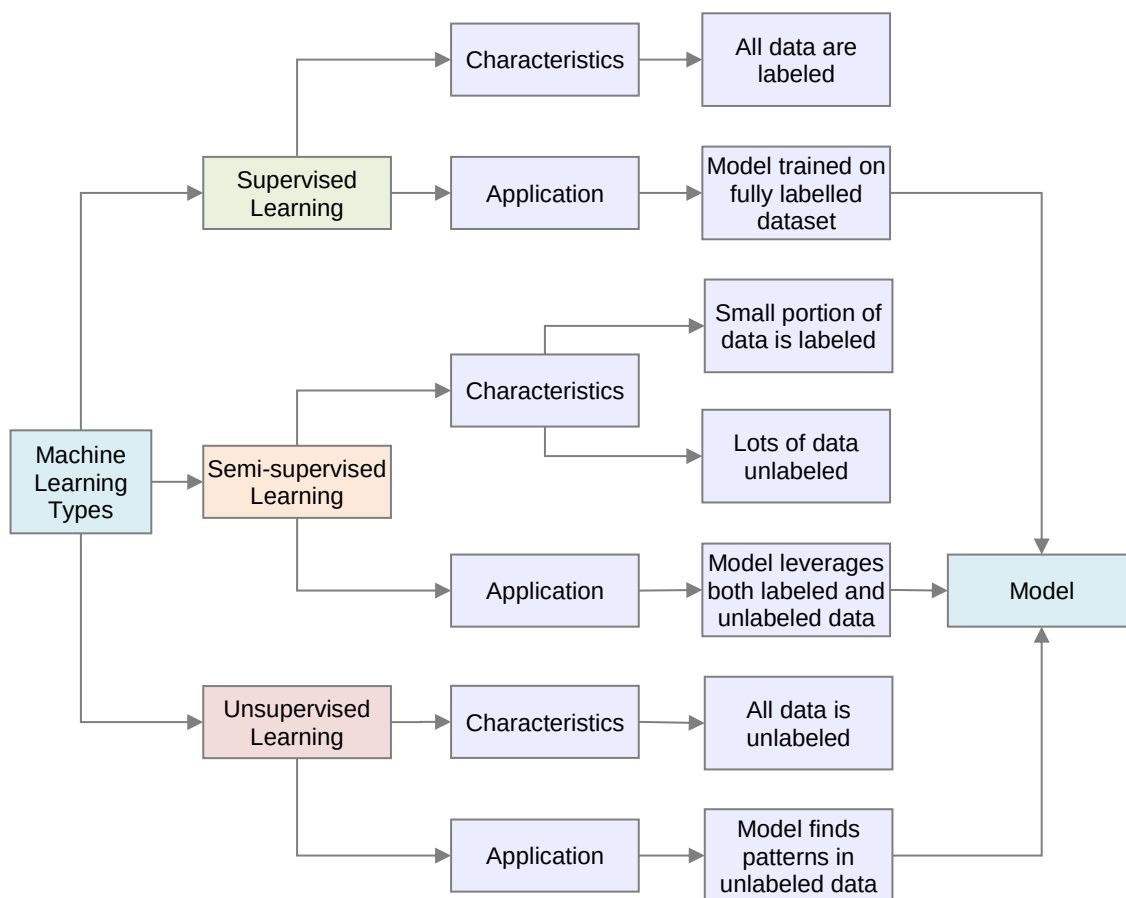


Figure 6. Taxonomy of machine learning approaches based on data labeling

3.1.1. Supervised Learning

Supervised learning is used to train models on labeled data, which helps solve problems like classification, regression, and prediction. Some of the most common algorithms used in this approach are linear regression, random forests, support vector machines (SVM), and neural networks [26,27]. These methods are widely used in many fields to get insights from structured and labeled data [28,29].

3.1.2. Unsupervised Learning

Unsupervised learning is a branch of machine learning that aims to analyze unlabeled data in order to discover underlying patterns, intrinsic structures, or meaningful groupings without prior knowledge of the target outputs (See figure 7). This method is especially helpful for things like clustering and reducing the number of dimensions.

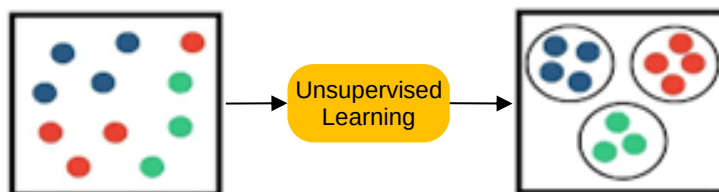


Figure 7. Unsupervised Learning

This method is especially helpful for things like clustering and reducing the number of dimensions. Some of the most popular algorithms are k-means, DBSCAN, principal component analysis (PCA), and

t-SNE [30,31]. These techniques facilitate the analysis of intricate data by recognizing inherent groupings or by streamlining data representation while maintaining its fundamental attributes [32,33].

Table 1 summarizes the main supervised and unsupervised learning algorithms, their characteristics, and typical application domains.

Table 1. Typical Algorithms in Supervised and Unsupervised Learning [18-20,24,34-36]

Learning Type	Algorithm / Technique	Description / Example Use Case
Supervised Learning	Linear Regression	Predicts a continuous output based on labeled data
	Logistic Regression	Predicts categorical outcomes
	Decision Tree	Classification or regression using hierarchical feature splits.
	Random Forest	Ensemble of decision trees to improve accuracy and reduce overfitting.
	Support Vector Machine (SVM)	Finds optimal boundary between classes for classification tasks.
	k-Nearest Neighbors (k-NN)	Predicts label based on closest neighbors in feature space.
Unsupervised Learning	k-Means Clustering	Groups data into clusters without labeled outcomes.
	Hierarchical Clustering	Builds tree-like clusters for exploratory data analysis.
	Principal Component Analysis (PCA)	Reduces dimensionality while preserving variance in data.
	Autoencoders	Learns compressed representations of data for feature extraction or denoising.

3.1.3. Semi-supervised learning

Semi-supervised learning improves model performance by using both labeled and unlabeled data. This is especially useful when there is not much labeled data available. This method is helpful for tasks like classification when there are not many labeled examples to work with. Some of the techniques used are autoencoders, which learn how to represent data in a way that saves space,

and label propagation methods, which automatically label data that does not already have a label based on data that does. These techniques utilize extensive volumes of unlabeled data to improve model accuracy and resilience [37,38].

Table 2 presents an overview of traditional machine learning algorithms employed for predictive analysis tasks.

Table 2. Traditional machine learning algorithms for predictive analysis [24,34]

Algorithm Type	Algorithm Name	Description / Use Case
Regression	Linear Regression	Predicts a continuous target variable based on linear relationships between features.
	Logistic Regression	Predicts a categorical outcome (binary/multi-class) using a logistic function.
Decision Trees	Decision Tree Classifier/Regressor	Tree-based model for classification or regression, splits data based on feature values.
Ensemble Methods	Random Forest	Ensemble of decision trees, reduces overfitting and improves prediction accuracy.
	Gradient Boosting (e.g., XGBoost)	Sequentially builds trees to correct errors of previous ones, highly effective for tabular data.
Instance-based Learning	k-Nearest Neighbors (k-NN)	Predicts based on the majority label (or average) of nearest data points in feature space.
Support Vector Machines	SVM Classifier / Regressor	Finds the optimal hyperplane to separate classes or predict continuous values.
Bayesian Methods	Naive Bayes	Probabilistic classifier based on Bayes' theorem, assumes feature independence.

3.1.4. Reinforcement Learning

The objective of reinforcement learning is to teach agents how to make decisions in a certain environment so that they can get the most rewards over time. This method can be used in many different fields, including gaming, robotics, and

process optimization. Some of the most popular algorithms are Q-learning, Deep Q-Networks (DQN), and Proximal Policy Optimization (PPO). These methods allow agents to learn by trying things out and making mistakes, which helps them get better over time [39,40].

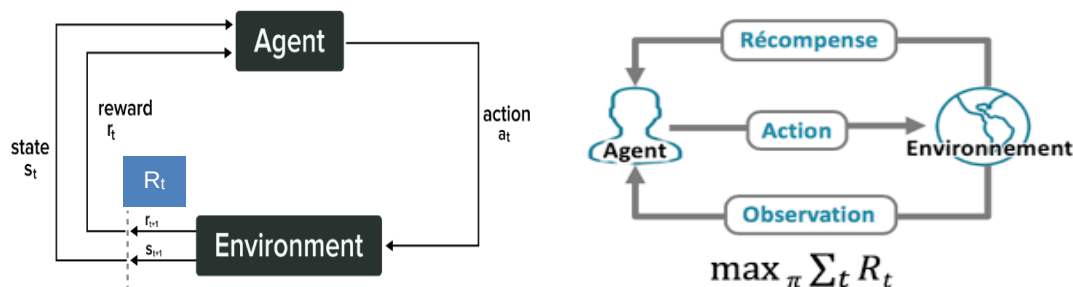


Figure 8. Mechanism of Reinforcement Learning

Figure 8 shows the basic idea of reinforcement learning: an agent learns best by trying things out and making mistakes in an environment, with a reward system that directs its learning toward getting the most long-term cumulative gain.

Figure 9 shows a typical data-driven workflow for materials science, focusing on how to create and use predictive models with traditional machine learning (ML).

The workflow is circular, which means that it goes from data to discovery and back again. There are four main steps to it:

1. Data Collection and Pre-processing (Top-Left): The process starts by getting data from three main sources: Experimental Data, Computational Data,

and Literature Data.

Action: This raw data is then put through a Data Cleaning & Normalization step to make sure it is of good quality and consistent before modeling.

2. Feature Engineering and Model Training (Top-Right): Action: Choose the most important features from the cleaned data. Training with Traditional ML is the most important part of this stage. The diagram shows Random Forest as an example of an algorithm used in this case.

3. Model Evaluation & Validation (Bottom-Right):

Action: The trained model's performance is carefully checked.

Tools: This includes methods like Cross-

Validation and keeping an eye on certain Performance Metrics like R^2 (coefficient of determination), MAE (Mean Absolute Error), and RMSE (Root Mean Square Error). The goal is to make sure that the model is correct and can be used with new data.

4. Deployment & Discovery (Bottom-Left):

Output: Once the model has been validated, it is deployed for its intended application materials

discovery and optimization. This stage, referred to as “Action,” involves using the trained model to generate predictions that can guide the identification of new materials or the enhancement of existing ones. The final step is Interpretation, where researchers analyze the model’s predictions to extract scientific insights. These insights may inspire new hypotheses and further data collection, thereby closing the loop and continuing the research cycle.

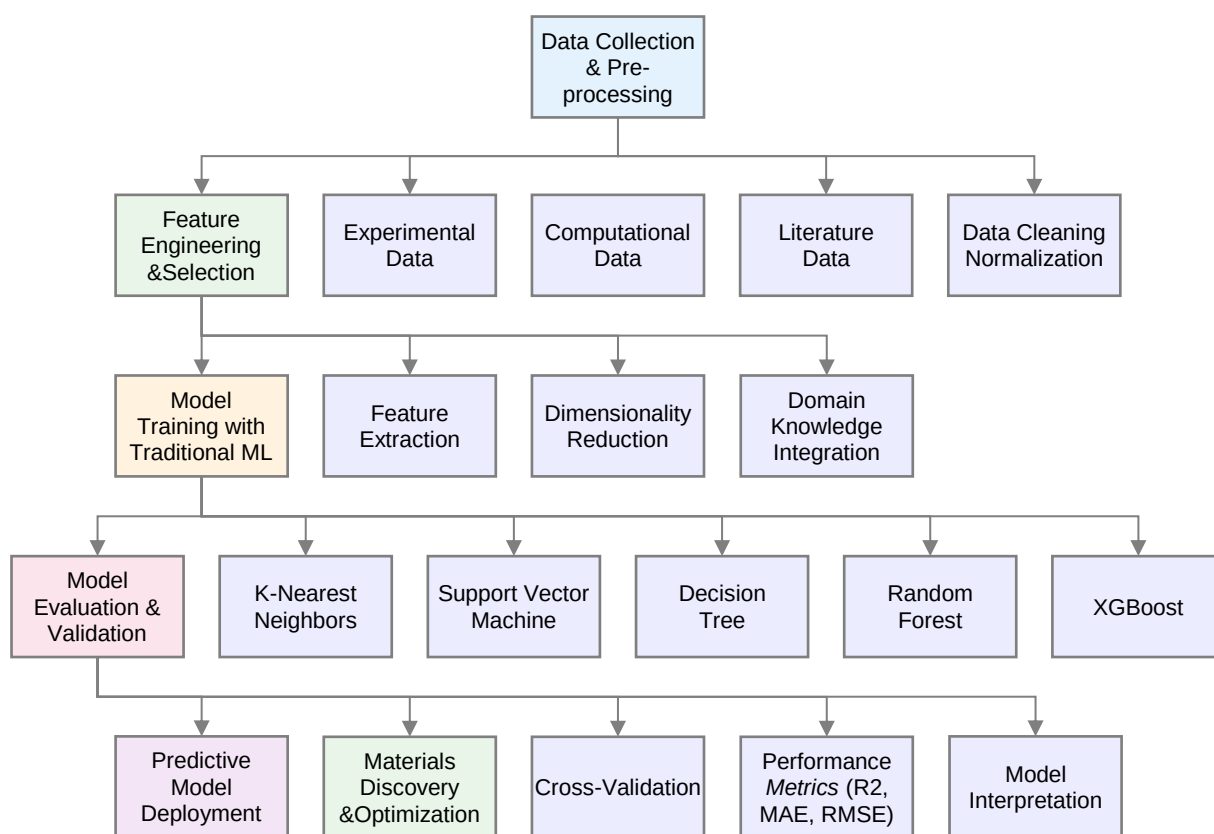


Figure 9. A typical data-driven workflow for developing predictive models in materials science using traditional machine learning

The choice of learning technique is driven by the nature of the problem and the type of data available in materials science. For instance, supervised learning serves as the cornerstone for building property prediction models (such as Young’s modulus or electrical conductivity) from existing databases, thereby reducing the need for costly experiments. Unsupervised learning, in contrast, plays a crucial role in uncovering hidden patterns or clusters within high-throughput characterization data (such as TEM images or XRD spectra), helping to identify new phases or microstructure–property relationships. Reinforce-

ment learning is proving to be transformative for optimizing dynamic and sequential processes, such as 3D printing parameters, where the agent learns to maximize part quality through simulated trial and error. The case studies presented in Sections 7.2 and 7.4 will illustrate these applications in detail.

3.2. Deep Learning

Deep learning is a type of machine learning that uses neural networks with many layers to model complicated data (See figure 10).

Many fields, like computer vision, natural language processing, and speech recognition, use

this method a lot. Convolutional Neural Networks (CNNs) for image analysis, Recurrent Neural Networks (RNNs) for temporal sequences, and Transformers for advanced natural language tasks

are some of the most popular architectures. These architectures are great at finding complex patterns and relationships in data, which is why they do well on certain tasks [41,42].

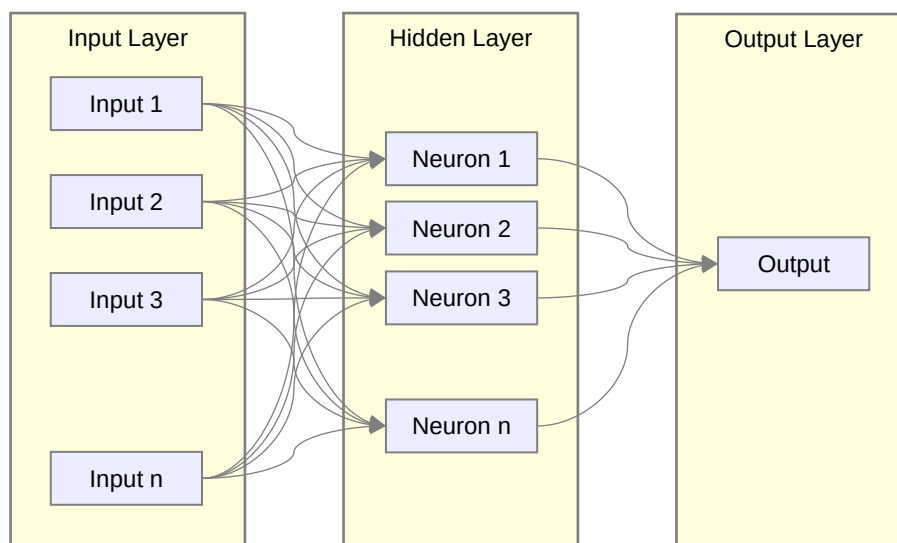


Figure 10. Architecture of a Fully Connected Feedforward Neural Network

Table 3 presents an overview of traditional deep learning algorithms employed for predictive analysis tasks.

Table 3. Commonly used deep learning models for predictive analysis

Algorithm Type	Algorithm Name	Description / Use Case
Feedforward Neural Networks (FNN)	Multilayer Perceptron (MLP)	Basic deep learning model with input, hidden, and output layers; used for regression and classification tasks.
Convolutional Neural Networks (CNN)	LeNet, AlexNet, VGG, ResNet	Specialized for grid-like data (e.g., images); captures spatial hierarchies using convolutional layers.
Recurrent Neural Networks (RNN)	Simple RNN, LSTM, GRU	Designed for sequential data; retains temporal information for time series, text, and speech analysis.
Autoencoders	Vanilla Autoencoder, Variational Autoencoder (VAE)	Unsupervised learning; learns compressed representations and reconstructs input data.
Generative Adversarial Networks (GAN)	DCGAN, StyleGAN	Consists of generator and discriminator; used for data generation, augmentation, and unsupervised tasks.
Deep Reinforcement Learning (DRL)	DQN, PPO, A3C	Combines deep learning with reinforcement learning; predicts optimal actions in dynamic environments.

3.3. Graph Neural Networks (GNNs)

Graph Neural Networks (GNNs) are designed to work with graph-structured data, which lets you model how nodes are connected and interact with each other [43,44]. People use these models a lot in fields like chemistry (to predict how molecules will behave), social networks (to look at how users interact with each other), and recommendation systems (to tailor suggestions to individual users based on their connections). Graph Convolutional Networks (GCNs) [35,36] and Graph Attention Networks (GATs) are two popular architectures that

use convolutions and attention mechanisms, respectively, to work with graph data. These methods get graphs to show complicated information and structural dependencies.

The efficacy of these techniques is not merely theoretical but is demonstrated in high-impact applications. Graph Neural Networks (GNNs), for example, have proven exceptional for predicting molecular crystal properties due to their inherent ability to model atomic bonds as graph structures, leading to accelerated discovery of organic

photovoltaic materials. Similarly, the optimization capabilities of Genetic Algorithms (GAs) are directly leveraged in the inverse design of high-entropy alloys, as detailed in Section 7.1.2, where they efficiently search vast compositional spaces to meet multi-property targets. These specific use cases bridge the gap between algorithmic description and practical utility.

3.4. Transfer Learning

Transfer learning is the process of using models that have already been trained on large datasets to do new tasks, especially when there is

not much data available for those tasks. A lot of people use this method in fields like computer vision and natural language processing (NLP). ResNet is a common pre-trained model for computer vision, and GPT and BERT are common pre-trained models for NLP. These models have already been trained on large datasets, so they can be adapted to specific tasks with only a small amount of extra data. This saves time, improves performance, and uses fewer resources [45] (See figure 11).

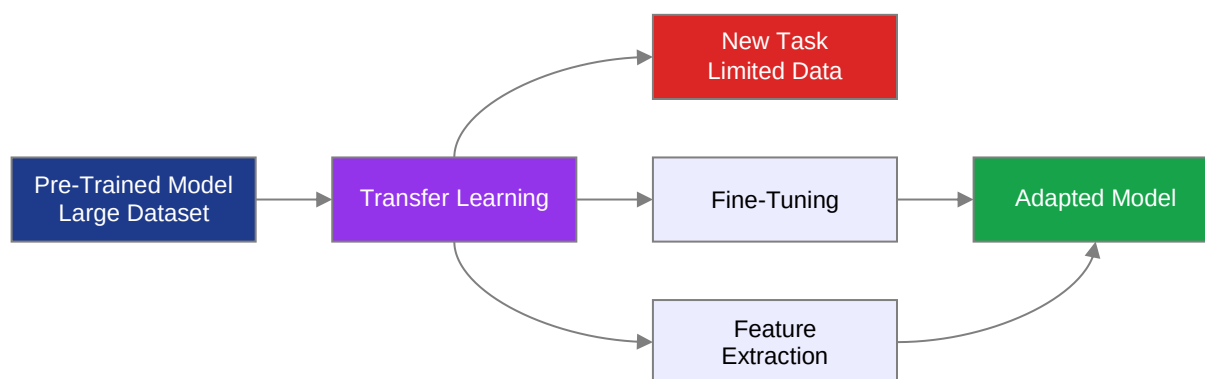


Figure 11. Transfer Learning Process

3.5. Federated Learning

Federated learning allows model training to happen on many devices at the same time, without compromising data privacy because the data stays on the users' devices. This method is especially helpful in sensitive areas like healthcare and the Internet of Things (IoT), where protecting data is very important [46,47]. Some examples of applications are Google's Gboard, which makes text prediction better while keeping user data private, and personalized recommendation systems. Federated learning enables the creation of robust models while preserving data confidentiality.

3.6. Swarm Intelligence and Genetic Algorithms

Nature-inspired optimization algorithms are methods that use natural events to find solutions to hard optimization problems. These techniques are used in a wide range of areas, including path planning and materials design. The ant colony algorithm, which uses the behavior of ants to find the best paths, and genetic algorithms, which are based on natural selection to find and improve

solutions, are two of the most famous examples. These methods are useful for solving hard problems that other methods might not work for [48,49].

Following all these cited techniques, we illustrate in the figure 12 the workflow for model development and evaluation. The process begins with an original dataset, which is split into a training set and a test set. The training set undergoes further splitting into a training subset and a validation set, where the model is trained and hyperparameters are tuned based on validation results. If the model achieves good performance during validation, it proceeds to final model evaluation using the unseen test set to estimate its true performance. This structured approach ensures that the model is rigorously assessed and generalizes well to new data before deployment.

3.7. Model Interpretability

In materials science, methods like SHAP (Shapley Additive Explanations) and Partial Dependence Plots (PDP) have been useful for figuring out how complicated ML models work. For example, when optimizing the recovery of rare earth elements from NdFeB magnets, SHAP

analysis showed how important calcination temperature, particle size, and acid concentration were to leaching efficiency. PDPs showed the best ranges for each parameter [34]. This blend of

global and local interpretability techniques lets researchers go from making predictions that are hard to understand to understanding how things work.

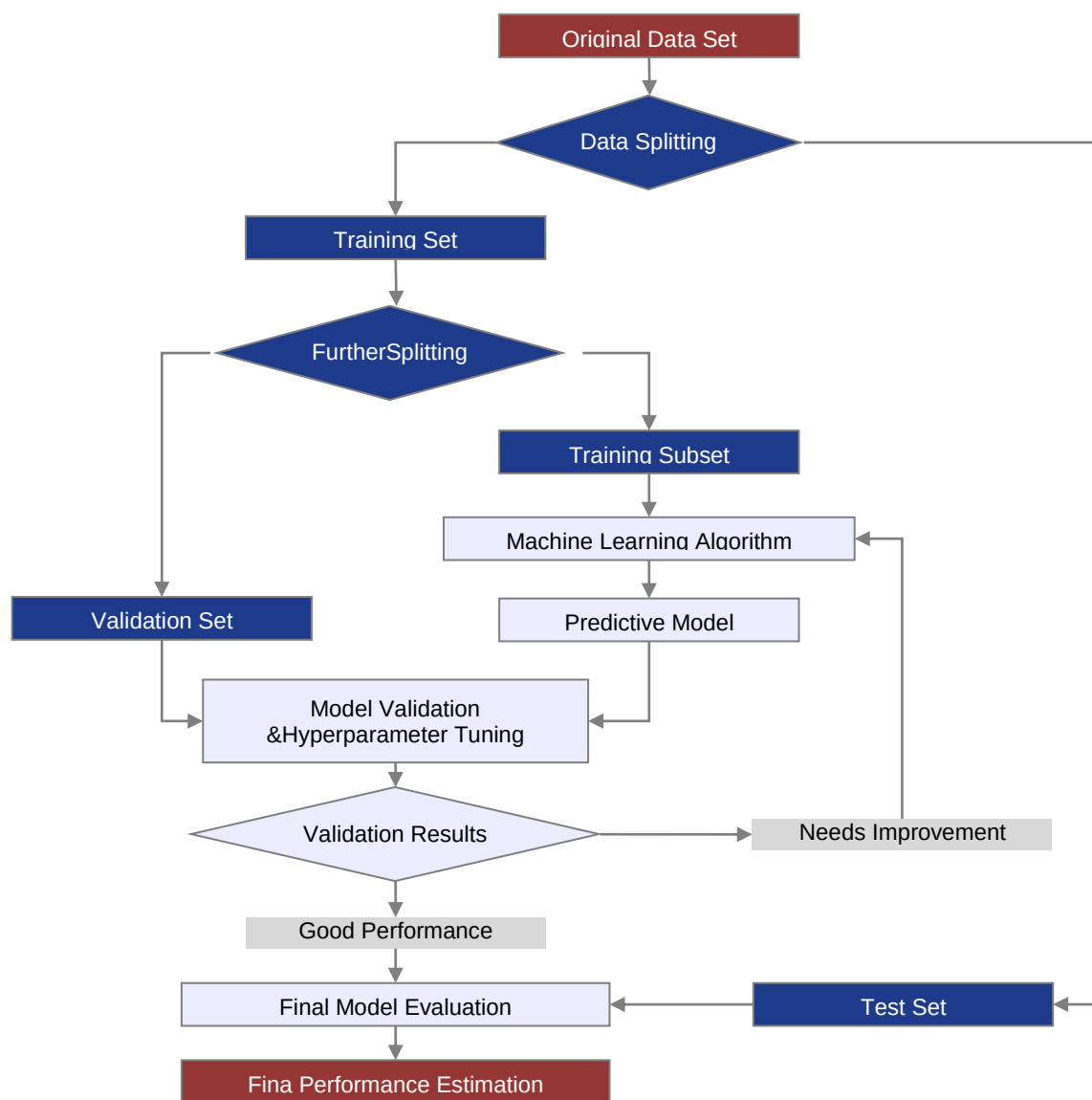


Figure 12. Workflow of dataset partitioning and model development process

4. AI TECHNIQUES COMMONLY USED IN MATERIALS SCIENCE

Machine learning, neural networks, and genetic algorithms are widely used AI techniques in materials science. Machine learning models such as linear regression, support vector machines (SVM), and random forests are commonly applied to predict material properties based on composition and processing parameters [26,50]. Deep learning architectures, including convolutional neural networks (CNNs) and recurrent neural networks (RNNs), enable the analysis of complex, high-dimensional data, with CNNs particularly suited for microscopy image analysis [51,52] and RNNs for

modeling time-dependent material behavior [53]. Genetic algorithms are employed to optimize material compositions and processing conditions by simulating evolutionary strategies to achieve target properties [54,55].

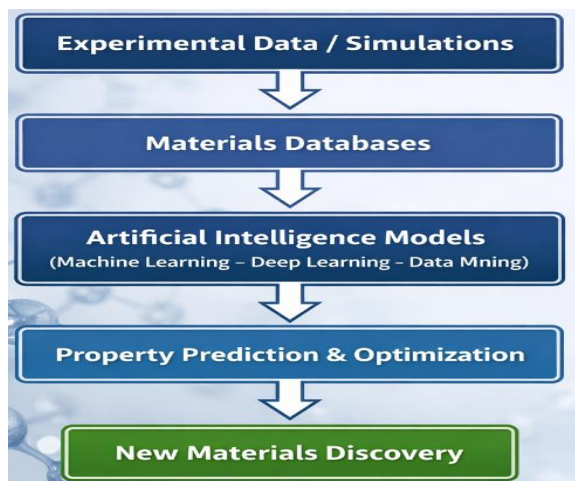


Figure 13. AI-Driven Workflow for the Prediction and Discovery of Novel Materials

The incorporation of artificial intelligence (AI) is transforming materials science by expediting the discovery and design of innovative materials (Figure 13). This change in thinking is backed up by basic reviews that show how machine learning

(ML) can change materials workflows [56,57]. Various AI methods show how this potential can be used: deep learning models predict the properties of alloys with better accuracy [58], genetic algorithms efficiently search compositional spaces [59], and graph neural networks provide understandable property predictions [7]. Moreover, deep learning methodologies are being developed for direct molecular design [60]. High-throughput computing and data mining are what make these methods work. They create the datasets that AI needs to make discoveries [11,61]. Together, these works create a strong, data-driven base for new materials.

Figure 14 illustrates the four paradigms of science and their progressive convergence toward predictive modeling, highlighting the integration of empirical, theoretical, and computational approaches with modern data-driven methodologies.

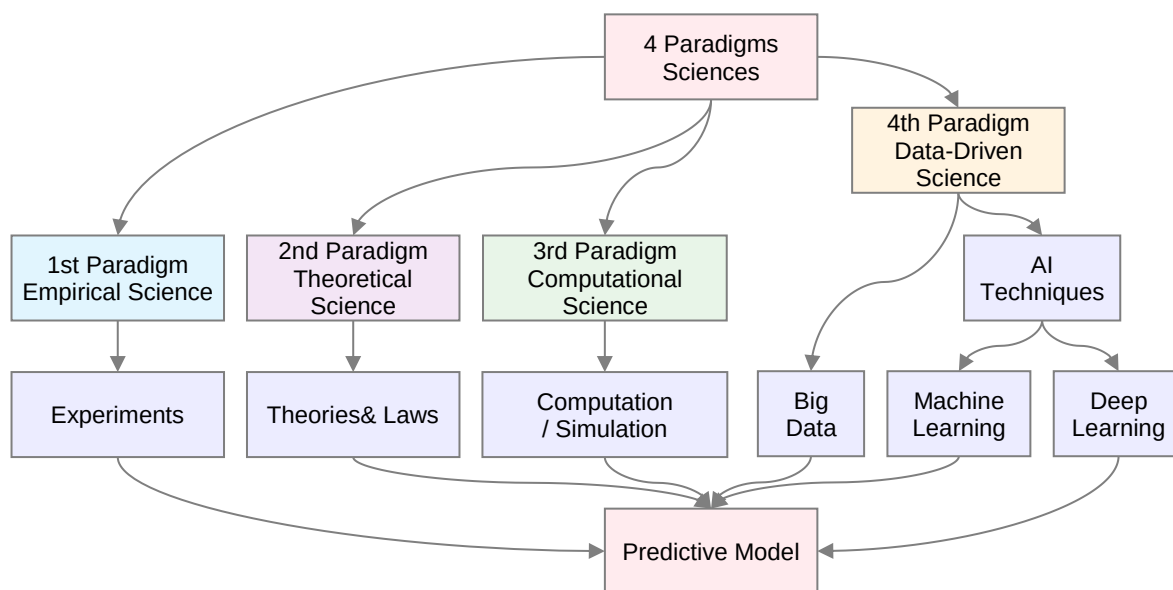


Figure 14. The four paradigms of science and their convergence toward predictive modelling, integrating traditional approaches (empirical, theoretical, computational) with modern data-driven science methods

5. GENERATIVE MODELS

Generative models are used to create new data that resembles a training dataset by capturing the underlying distributions of existing data [62,63]. These models find applications in various fields such as image creation, text synthesis, and molecule design. Among the most popular examples are GANs (Generative Adversarial Networks), which use two competing neural networks (a generator and a discriminator) to

produce realistic data, and VAEs (Variational Autoencoders), which learn a latent representation of data to generate new instances. These techniques enable the production of innovative and high-quality content.

Figure 15 illustrates the transformative impact of Generative Artificial Intelligence (GAI) on materials science, highlighting its diverse applications across the materials development pipeline. GAI enables accelerated materials

discovery through de novo design of crystals, molecules, and alloys, while also predicting complex material properties with high accuracy. In process synthesis and manufacturing, it optimizes reaction conditions and manufacturing parameters, bridging the gap between laboratory synthesis and industrial-scale production. GAI also improves materials characterization by interpreting spectroscopic data and looking at microstructures, which gives researchers a better understanding of their experimental results. This comprehensive integration of generative models throughout the materials science workflow demonstrates their potential to revolutionize traditional research methodologies, enabling faster, more efficient, and data-driven approaches to materials innovation and development.

These generative capabilities have direct and transformative implications for materials design. For example, conditional Generative Adversarial Networks (GANs) have been specifically trained to

propose new organic molecules for photovoltaic cells [64].

Several of the AI-designed molecules that were subsequently synthesized achieved power conversion efficiencies (PCE) exceeding 10% in laboratory tests. This demonstrates the ability of generative models to explore chemical spaces far beyond human intuition and to deliver viable candidates for energy applications[64,65].

Generative AI identifies grain size and grain boundaries primarily through semantic segmentation using models like GANs and Denoising Diffusion Probabilistic Models (DDPMs) that learn to generate boundary masks from microscopy images, achieving accuracy exceeding 95%. These models are trained on paired datasets (e.g., SEM images with EBSD ground truth) to differentiate grain interiors from boundaries, enabling precise microstructural quantification.

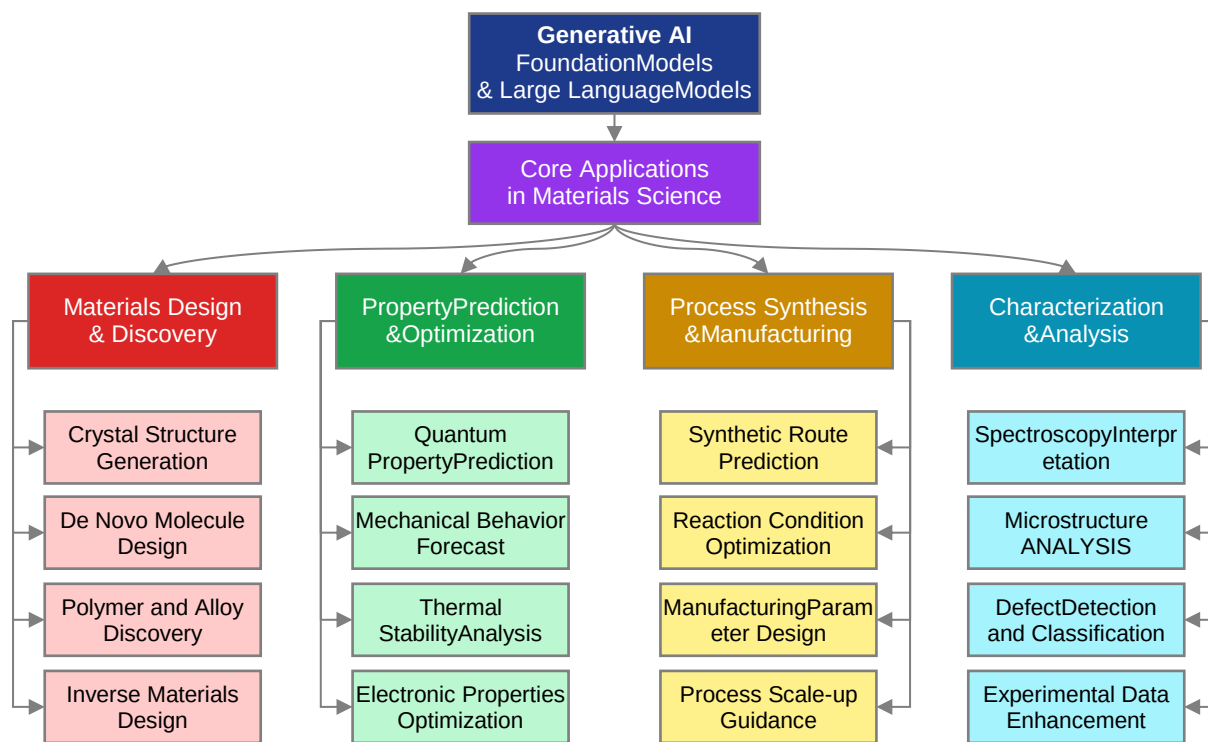


Figure 15. GAI and its application in materials science

6. PHYSICS-INFORMED NEURAL NETWORKS (PINNS)

Physics-Informed Neural Networks (PINNs) are a new way for artificial intelligence to use physical knowledge directly in neural networks [66,67]. PINNs are different from regular neural networks because they use governing equations (Figure 16), initial and boundary conditions, or other physical constraints in the training process [68]. This allows

the network to respect the underlying physics of the system while learning from data, improving generalization and reducing the need for large datasets [69]. PINNs have been effectively utilized in various domains, including fluid dynamics, heat transfer, structural mechanics, and material science, facilitating the resolution of both forward and inverse problems governed by partial differential equations [70,71]. PINNs combine

domain knowledge with machine learning to create a powerful framework for modelling complicated physical systems with better accuracy and dependability.

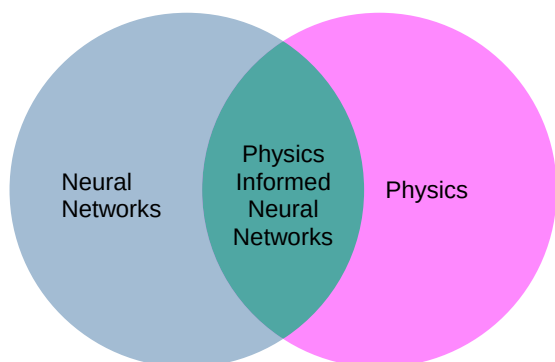


Figure 16. Concept of PINNs

Concept of PINNs

PINNs combine:

- Neural Networks: To learn models from data.
- Physical Knowledge: By integrating differential equations or physical constraints directly into the network's loss function.

This approach enables the solution of problems

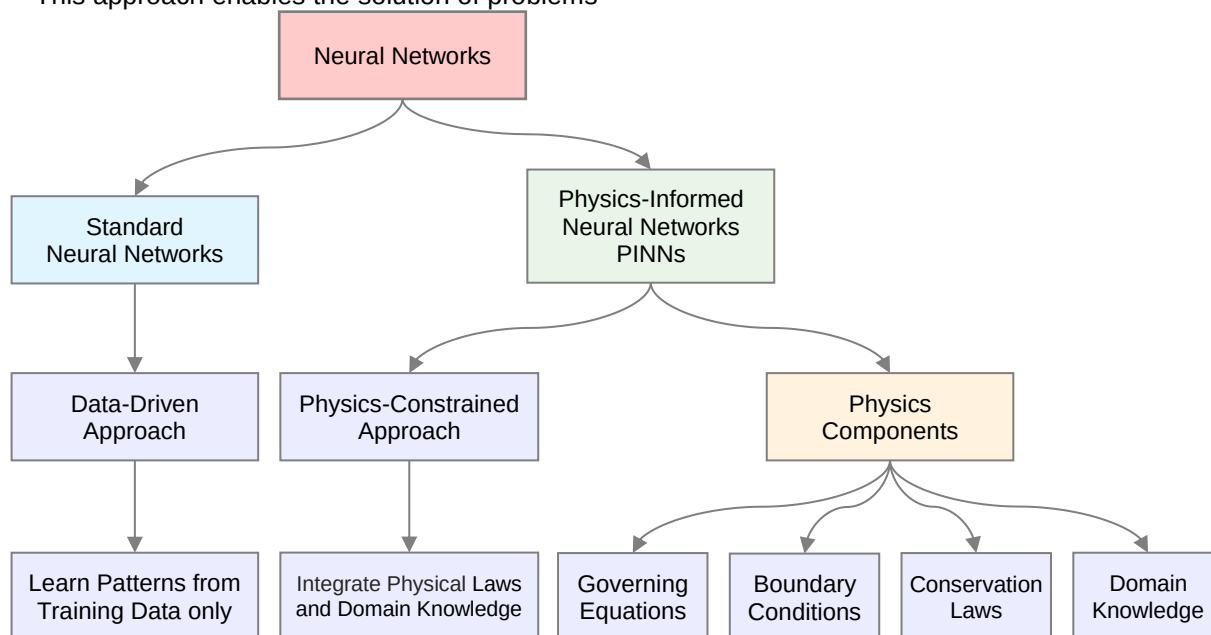


Figure 17. Comparison between standard Neural Networks and Physics-Informed Neural Networks (PINNs)

6.1. Neural Network Architecture

- A neural network is used to approximate the solution to a physical problem. This network takes input variables (such as time, space, or other parameters) and produces outputs (such as temperature, pressure, or velocity fields).
- The network is trained to minimize a loss

where data is scarce or noisy, while ensuring that the solutions satisfy the underlying physical laws.

Figure 17 shows the main difference between regular Neural Networks and Physics-Informed Neural Networks (PINNs). Traditional neural networks function solely as data-driven models, acquiring patterns exclusively from the training dataset. In contrast, Physics-Informed Neural Networks (PINNs) incorporate essential physical domain knowledge. This hybrid architecture incorporates physical constraints, including governing equations, boundary conditions, and conservation laws, directly into the learning process. PINNs use these physics-based parts to make sure that the model's predictions are not only consistent with the data but also follow the system's basic physical laws. This makes the scientific models stronger, easier to understand, and more applicable to other situations.

Physics-Informed Neural Networks (PINNs) work by using a new way to combine neural networks and physical knowledge to solve scientific and technical problems. The most important steps in how they work will be provided below.

6.2. Integration of Physical Laws

- Differential equations or physical constraints (such as conservation laws or partial differential equations) are integrated directly into the loss function.

- b. For example, if the physical equation is $F(u) = 0$, where u is the sought solution, the neural network is constrained to minimize $F(u)$ in addition to the error on the observed data.

6.3. Composite Loss Function

The total loss function is a combination of two terms:

$$l = l_{data} + \lambda \cdot l_{physic}$$

Where λ is a hyperparameter that weights the importance of the physical constraints.

- Data term: Measures the discrepancy between the network's predictions and the observed data (when available).
- Physics term: Measures how well the network's predictions satisfy the physical equations.

6.4. Network Training

The network is trained using optimization methods like gradient descent to minimize the composite loss function. The derivatives needed to

evaluate the physical terms (such as partial derivatives) are efficiently calculated through automatic differentiation.

6.5. Key Advantages

Sparse or noisy data: PINNs can work with limited data, as physical laws guide the learning process.

Physically plausible solutions: The solutions respect physical constraints, even in the absence of data.

Flexibility: PINNs can be applied to a wide variety of problems, including nonlinear partial differential equations (PDEs) and complex systems.

6.6. Typical Applications

- Solving differential equations
- Modeling physical phenomena (fluid mechanics, heat transfer, etc.)
- Inverse problems (parameter estimation from observed data)

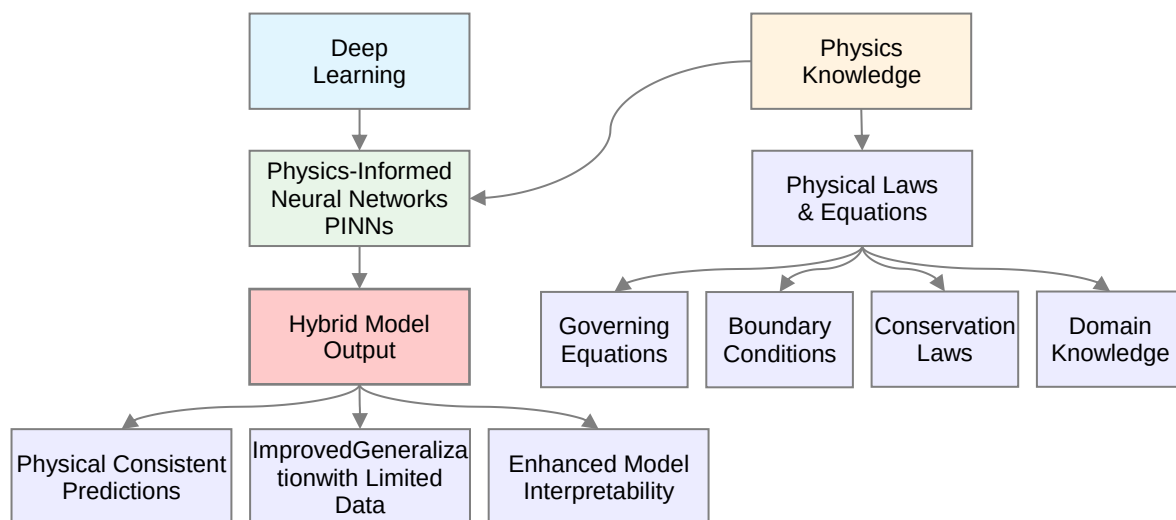


Figure 18. Integration of deep learning with physics knowledge through Physics-Informed Neural Networks (PINNs)

Figure 18 shows how Physics-Informed Neural Networks (PINNs) can combine deep learning and basic physics knowledge in a very powerful way. This framework signifies a paradigm shift from exclusively data-driven methodologies by methodically integrating physical laws and constraints, such as conservation laws, boundary conditions, constitutive relations, and governing equations, directly into the neural network architecture. PINNs create hybrid models that make predictions that are consistent with physics while still keeping the expressive power of deep learning by incorporating this physics-based

knowledge. This integration has a number of important benefits, such as better prediction accuracy that takes physical limits into account, better generalization even with little training data, and better model interpretability by making domain knowledge explicit. The resulting models are especially useful in science and engineering where physical consistency is very important. They fill the gap between traditional mechanistic modelling and modern data-driven AI methods.

Physics-Informed Neural Networks (PINNs) are utilized across various disciplines, including engineering for fluid simulation, thermodynamics,

and structural mechanics; materials science for predicting material properties and modelling physical processes; geophysics for simulating earthquakes and subsurface flows; biology for modelling intricate biological systems; and finance for resolving stochastic differential equations in option pricing. These applications show how flexible PINNs are in combining physical laws with neural network-based models, which makes it possible to solve hard problems in many different situations [72].

Physics-Informed Neural Networks (PINNs) have a number of important benefits. For example, they use physical knowledge to reduce the need for a lot of data, which is useful when there is not much data available. They also make solutions easier to understand by ensuring that they follow the rules of physics, which makes them more believable. They can be used to solve a wide range of physical problems, from differential equations to complex systems, and they are often more efficient than traditional numerical methods, especially for problems where solutions can be found with fewer computational resources. These traits make PINNs a great way to model and solve scientific and technical problems.

In materials science, Physics-Informed Neural Networks (PINNs) have proven especially valuable for modeling complex phenomena where experimental data are scarce or expensive to obtain [73].

By directly embedding thermomechanical equations (such as Fourier's law and Hooke's law) into the neural network's loss function, the PINN model was able to accurately predict temperature and strain fields across the weld, using only a handful of thermal data points for training.

These predictions made it possible to optimize welding parameters (speed and power), reducing distortion by more than 50% compared with the initial empirical settings. This approach offers a valuable and significantly faster alternative to traditional finite element simulations for tackling such coupled multiphysics problems [73].

7. APPLICATIONS OF AI IN MATERIALS SCIENCE

AI has changed many fields, including materials science, in a great way (See figure 19). The use of AI in this field has sped up the discovery of new materials, improved the properties of existing materials, modelled and simulated how materials behave, and improved manufacturing and production processes [74].

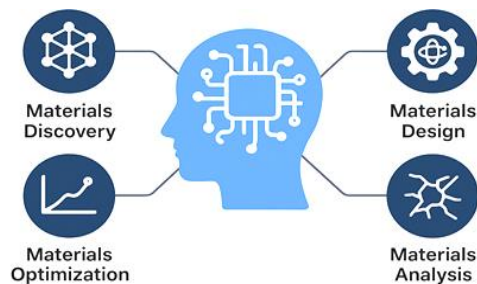


Figure 19. Summary of AI applications in materials science

Accelerating Material Discovery: AI helps researchers quickly find and design new materials by looking at large sets of data and making predictions about material properties. Machine learning algorithms can look through millions of possible material combinations, which saves a lot of time and money compared to traditional experimental methods [75,76]. AI methods like neural networks and genetic algorithms are used to improve the properties of materials. AI can suggest changes to get the desired properties, like improved strength, conductivity, or durability, by looking at how composition, structure, and performance are related [75,77].

Modelling and Simulation: AI makes it easier and more accurate to model and simulate materials. Deep learning and other methods can tell us how materials will act in different situations, like when they are under stress, at high temperatures, or exposed to chemicals [75,77]. This is especially useful in fields like aerospace, energy, and biomedicine, where materials have to meet very high standards for performance.

Improving Manufacturing Processes: AI makes manufacturing better by controlling production parameters in real time, cutting down on waste, and making products better. For instance, AI-driven systems can change the way things are processed to make sure they are always the same and accurate, which leads to higher yields and lower costs [75,78].

These applications show how AI is changing the field of materials science by speeding up innovation, making processes more efficient, and creating advanced materials with tailored properties. Researchers and industry can push the limits of what is possible in materials science by using AI.

Classification techniques like Random Forest are used for rapid screening of battery materials, predicting suitability with up to 96% accuracy from chemical formulas alone. Bayesian Optimization enables efficient exploration of enormous composition spaces (millions of candidates) by

balancing multiple electrochemical properties simultaneously with minimal experimental data. Inverse design approaches such as Particle Swarm Optimization (PSO) and Genetic Algorithms combined with Neural Networks identify specific elements and manufacturing conditions to achieve target properties like capacity retention. Surrogate models including XGBoost ($R^2=0.83$) and Deep Kernel Learning serve as predictive cores for these optimization frameworks, enabling physics-informed digital design and accelerating the discovery of optimal battery compositions.

7.1. Discovery of New Materials

Finding new materials is a hard and expensive job that has always depended on trial and error. AI speeds up this process by using machine learning algorithms to look at large datasets and find promising compositions [79-81].

Examples of success in finding new materials:

- **High-entropy alloys:** Researchers at the University of California, Berkeley, used neural networks to find new high-entropy alloys. Their method found alloy compositions with the best mechanical and thermal properties, which cut down on the time and money needed for traditional methods by a large amount [79,82].
- **Battery Materials:** Another example is finding new materials for the cathodes of lithium-ion batteries. Researchers used machine learning to predict how different chemical compositions would work, which led to the discovery of materials that can store more energy and last longer.
- **Polymer Materials:** In the area of polymers, deep learning models have been used to find new materials with certain characteristics, like being flexible and able to withstand heat. These findings may be useful in the fields of flexible electronics and packaging [80].

7.1.1. Case Study: Discovery of Novel Solid-State Electrolytes for Li-ion Batteries

A compelling example of AI-accelerated materials discovery is the identification of new lithium solid-state electrolytes (SSEs). These materials are essential for developing safer batteries with higher energy density, yet exploring the vast chemical space of potential candidates through conventional trial-and-error methods is prohibitively slow [79].

In a landmark study, researchers implemented a machine learning (ML) pipeline combining a random forest classifier and a gradient boosting regressor (XGBoost) to screen more than 12,000 lithium-containing compounds extracted from materials databases such as the Materials Project [6,80].

The ML models were trained to predict two key properties: structural stability (i.e., the likelihood of being a viable SSE) and lithium-ion conductivity. The initial screening highlighted $\text{Li}_6\text{PS}_5\text{Cl}$, a member of the argyrodite family, as a leading candidate, with both high predicted stability and a favorable conductivity window.

Subsequent density functional theory (DFT) calculations, followed by experimental synthesis, validated the model's predictions. The measured room-temperature ionic conductivity exceeded 1 ms/cm , a value suitable for practical applications [80].

By adopting this AI-first strategy, the researchers reduced the initial screening timeline from years to just weeks. More importantly, the approach directly enabled focused experimental efforts on a now-promising class of electrolytes, demonstrating an efficient pipeline that moves seamlessly from virtual screening to experimentally realized materials [79,80].

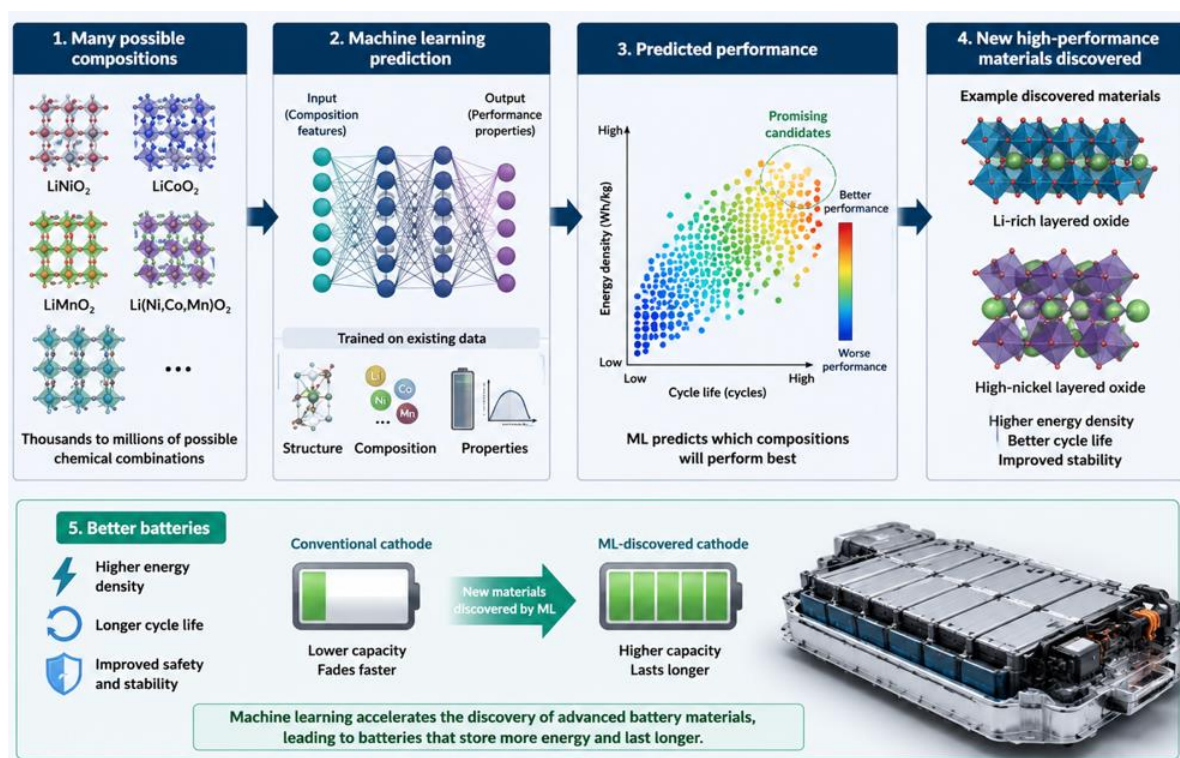


Figure 20. Machine Learning for Advanced Battery Material Discovery

Figure 20 illustrates the ML-enabled workflow for the discovery of advanced battery cathode materials, where ML models are used to predict performance properties (energy density and cycle life) from compositional features to screen thousands of candidates. The approach successfully discovers new materials such as Li-rich layered oxides with enhanced energy density, cycle life, and stability, leading to batteries with enhanced performance compared to conventional cathodes.

7.1.2. Case Study: Designing High-Entropy Alloys with Targeted Mechanical Properties

Designing high-entropy alloys (HEAs) with both high mechanical strength and good ductility is a challenging multi-objective optimization problem. To tackle this, researchers combined a genetic algorithm (GA) with a deep neural network (DNN) surrogate model [83-85].

The DNN was first trained on an existing dataset of HEA compositions along with their experimentally measured properties, such as yield

strength and elongation. Once trained, the genetic algorithm generated successive populations of candidate compositions. Instead of fabricating and testing each alloy, the DNN rapidly predicted the fitness of thousands of virtual candidates—specifically evaluating the strength–ductility trade-off—thereby avoiding costly and time-consuming experiments.

This iterative loop converged on an optimal compositional region centered around $\text{Al}_{0.5}\text{CoCrFeNiTi}_{0.2}$. Alloys synthesized following this AI-guided strategy exhibited an approximately 15% increase in yield strength (reaching about 950 MPa) while maintaining elongation above 20%, effectively overcoming the traditional strength–ductility trade-off.

This example highlights the power of AI-driven inverse design: instead of measuring properties after synthesis and adjusting incrementally, the desired properties directly steer the search for the optimal composition.

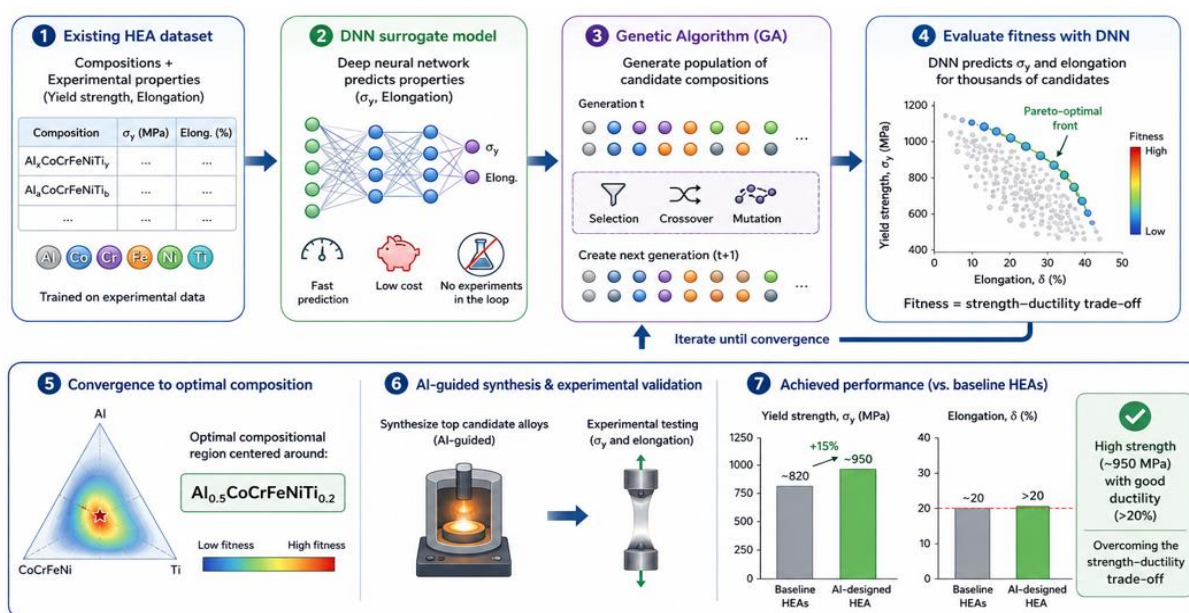


Figure 21. AI-Driven Inverse Design of High-Entropy Alloys with Targeted Mechanical Properties

Figure 21 illustrates the AI-driven inverse design framework for high-entropy alloys, integrating a deep neural network surrogate model with a genetic algorithm to optimize the strength-ductility trade-off.

7.2. Optimization of Material Properties

Another important use of AI is to improve the properties of materials that are already there. Machine learning algorithms can find and change processing parameters to improve the properties of materials [86-88].

Examples of AI-Optimized Material Properties:

- Mechanical Properties of Composites:** AI has been used to improve the mechanical properties of fiber-reinforced composites in the composites industry. Researchers made composites stronger and longer-lasting by changing the resin-to-fiber ratios and curing conditions, for example [87].
- Enhancement of Ceramic Materials:** Scientists have also used AI to make ceramic materials better. Machine learning algorithms improved the fracture resistance and thermal conductivity of ceramics by changing the chemical compositions and sintering conditions [88].
- Thermal Properties of Alloys:** AI methods have been used to improve the thermal properties of metal alloys. Researchers improved thermal conductivity and oxidation resistance by changing the composition of alloys and the conditions under which they were heated [86].

These examples show how AI is changing materials science by making it possible to find new materials faster, make them more precise, and create new materials that are better suited for certain uses [86-88].

7.2.1. Case Study: Optimizing the Fracture Toughness of Ceramics with AI

Optimizing technical ceramics, such as yttria-stabilized zirconia (YSZ) for biomedical applications (e.g., implants) or energy devices (e.g., fuel cell electrolytes), requires precise control over microstructure. A machine learning approach was employed to maximize the fracture toughness (K_{1c}) of YSZ by simultaneously optimizing multiple sintering parameters [89,90].

A random forest regression model was trained on historical data linking processing parameters such as sintering temperature, duration, applied pressure, and initial powder size to measured mechanical properties. The model then guided a sequential experimental campaign using Bayesian optimization. This approach intelligently explored the parameter space to identify a global optimum.

The optimal protocol identified sintering at 1450°C for 120 minutes under a specific pressure produced a fine and uniform grain microstructure. Samples processed under these conditions exhibited a nearly 30% increase in fracture toughness (from ~4 to ~5.2 $\text{MPa}\cdot\text{m}^{1/2}$) compared to the standard protocol, without compromising density.

This case clearly demonstrates how AI can go

beyond empirical expertise to uncover complex process-structure-property relationships, achieving superior material performance.

7.2.2. Case Study: Targeted Improvement of Polymer Composite Properties

In the field of composite materials, optimizing the fiber-matrix interface is critical. One study employed convolutional neural networks (CNNs) to automatically analyze scanning electron microscopy (SEM) images of carbon fiber-epoxy composites [91]. The CNN was trained to quantify microstructural descriptors such as fiber/matrix adhesion, porosity, and fiber distribution and

correlate them with measured mechanical strength.

The model revealed that fiber surface roughness and a specific polymer functionalization ratio were the most predictive microstructural factors for interlaminar strength. By guiding surface chemical modifications of the fibers and selecting coupling agents based on these insights, the interlaminar strength of the composite was increased by 25%, from 40 to 50 MPa.

“image-to-property” approach highlights the potential of AI to understand and optimize material properties directly from their fundamental microstructure (See figure 22).

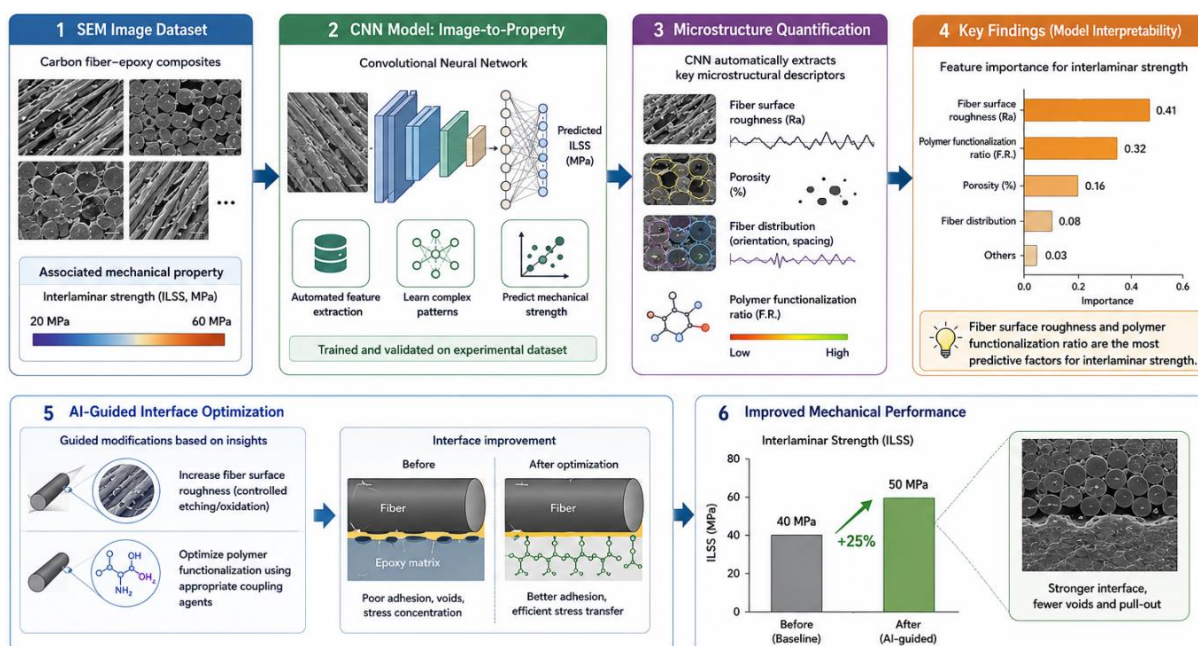


Figure 22. AI-Driven optimization of polymer composite properties

7.3. Modelling and Simulation

AI is very important for modelling and simulating how materials behave. Researchers can use machine learning-based predictive models to simulate how materials will behave in different situations, which helps them understand how well they work [92-94].

The part AI plays in modelling how materials act and what they are made of Neural networks have been used to model how materials behave mechanically when they are under stress. These models show how materials change shape and break under different loads, which is important for design and manufacturing [92].

AI has also been used to model the electronic properties of materials, like semiconductors. Researchers can use predictive models to figure out how fast charge carriers can move and how wide the bandgaps are. These are very important

for making electronic devices [93]. AI can also be used to model how materials behave when they are heated, researchers can improve the compositions of materials for certain uses, like heat sinks and thermal insulators, by simulating how heat moves through and around them [94]. These applications show how AI makes it easier to predict and understand how materials behave, which makes it possible to design materials with specific properties for advanced technologies.

7.4. Fabrication and Production

AI is being used more and more to improve the processes designed to make and produce materials. AI can lower costs, make things more efficient, and make sure that materials are of higher quality by optimizing production parameters and keeping an eye on the quality of finished goods [92-94].

Additive

Manufacturing

Process

Optimization: AI is used to improve printing settings in additive manufacturing (3D printing), such as the speed of extrusion and the temperature of the nozzle. These improvements make it possible to make parts that are more accurate in size and have better mechanical properties [92]. Machine learning algorithms such as Random Forest, Support Vector Machines (SVM), and Gradient Boosting (XGBoost) can be implemented to optimize print settings by learning the relationships between process parameters (e.g., temperature, speed, layer height) and final part quality metrics (e.g., dimensional accuracy, surface roughness, mechanical strength). Bayesian Optimization is particularly effective for this purpose, as it intelligently explores the parameter space to find optimal settings with minimal experimental trials, reducing material waste and production time. Reinforcement Learning and Deep Neural Networks can also be used for real-time adaptive control, enabling closed-loop adjustment of print parameters during the printing process to compensate for defects or variations in material properties.

Quality Control in Real Time: AI systems are also used to check the quality of materials as they are being made. Computer vision and image processing algorithms can find and fix defects right away, which lowers rejection rates and production costs [93].

AI is used for predictive maintenance of production equipment, by looking at sensor data and using machine learning algorithms, it is possible to predict failures before they happen. This lets you plan maintenance work and keep downtime to a minimum [94].

These applications show how AI is changing the way things are made and produced, making them faster, cheaper, and more reliable while also making sure that high-quality materials are made.

7.4.1. Case Study: Real-Time Control and Optimization of a Metal Additive Manufacturing Process

Metal additive manufacturing is highly sensitive to defects such as porosity, which can compromise mechanical properties [92,94]. One study implemented an AI-based closed-loop control system for a Laser Powder Bed Fusion (LPBF) process [95].

Optical and thermal sensors monitored the powder fusion in real time. The data including images of the melt pool and temperature readings were processed by a lightweight convolutional neural network (CNN) trained to detect anomalies that could lead to porosity, such as underfusing or balling. When a defect was predicted, the system

instantaneously adjusted the laser parameters (power, speed) to correct it.

In the fabrication of stainless steel 316L parts, this approach reduced the average porosity rate from 0.5% to less than 0.1% and decreased property variability. Most notably, the scrap rate dropped from 12% to under 3%, delivering substantial economic benefits.

This case demonstrates the shift from passive monitoring to adaptive, AI-driven resilient manufacturing.

7.4.2. Case Study: Predictive Maintenance in an Aluminum Rolling Mill

Unexpected production line stoppages are costly. In an aluminum rolling mill, a predictive maintenance approach using machine learning was implemented on critical mill bearings [96]. Multivariate data including vibrations, temperature, load, and acoustic signals were continuously collected from the equipment.

An unsupervised learning model, based on the Isolation Forest algorithm, analyzed these data streams to detect subtle deviations from normal operation, often imperceptible to human operators. When an anomaly was detected, the system estimated both the probability of failure and the expected time horizon, enabling maintenance interventions to be scheduled during planned downtime.

Implementation of this system resulted in a 65% reduction in unplanned failures on the monitored equipment and extended the average service life of the bearings by 40%. This case demonstrates how AI can transform maintenance from a costly calendar-based program into a condition-based strategy grounded in the real-time state of equipment.

7.5. AI-Driven Process Optimization in Materials Recycling

A recent study on NdFeB magnet recycling demonstrates the power of ML in optimizing hydrometallurgical processes [34]. The researchers developed ML models incorporating 24 input parameters including particle size, waste composition, calcination parameters (time, temperature), and acid leaching parameters (pulp density, stirring speed, acid type and concentration) to predict the leaching efficiency of rare earth elements (Nd, Dy, Pr) as well as Fe and Co. Among the algorithms tested (XGBoost, Random Forest, SVM, and AdaBoost), XGBoost demonstrated the highest prediction accuracy using 5-fold cross-validation on a dataset of 9,650 points. The optimized conditions (60 min leaching time, 95°C temperature, 125 g/L solid-to-liquid ratio) achieved REE recovery efficiencies with errors below 5% between predicted and

experimental values.

8. INTERDISCIPLINARY COLLABORATION AND FUTURE RESEARCH OPPORTUNITIES

To advance this interdisciplinary field, materials scientists and artificial intelligence (AI) experts must work closely together. Collaboration is essential to develop AI models tailored to the specific needs of materials research. For instance, making databases of material properties openly accessible enables more effective training of AI models [97,98]. Similarly, combining machine learning with quantum mechanics calculations improves the accuracy and reliability of property predictions [97,99]. To ensure reproducibility and trustworthiness of results, it is crucial to establish standardized protocols and norms for the application of AI in materials science [97,100].

A successful example of such interdisciplinary collaboration is the materials informatics pipeline for solid-state electrolyte discovery (Section 7.1.1). In this workflow, data scientists developed and trained machine learning models on curated databases, computational materials scientists validated predictions with DFT calculations, and experimental synthesis experts characterized the final compounds. This seamless integration across disciplines compressed the development timeline from years to months, highlighting that interdisciplinary teams are essential to fully realize AI-driven materials innovation.

A new generation of researchers proficient in both AI and materials science is needed [99]. Additionally, international and interdisciplinary collaborative initiatives are critical for addressing complex challenges, such as discovering materials for clean energy or personalized medicine [98,100]. The use of open data, as promoted by initiatives like the Materials Project or the Materials Genome Initiative, accelerates discoveries by facilitating data sharing across institutions and countries [97,98]. These combined efforts are paving the way for significant advances in AI-driven materials science.

9. APPLICATIONS OF AI IN MATERIALS SCIENCE: QUANTITATIVE INSIGHTS

The use of AI has led to measurable improvements in the workflows for finding new materials [101,102]. High-throughput virtual screening methods now allow for the testing of

more than 100,000 potential materials every day [103]. This is 100 times faster than traditional experimental methods. Neural network models have been able to predict phase stability with 92% accuracy in the search for metal alloys. This has cut the costs of experimental validation by about 75%. Machine learning classifiers can find promising cathode compositions for battery materials with 88% accuracy [102,104], which cuts down on failed synthesis attempts by 60% [64,65,73,82,101-104].

AI-driven optimization has led to statistically significant changes in the properties of materials. Gradient boosting algorithms have improved the mechanical properties of polymer composites by 15–25% in tensile strength and 8% in density. Bayesian optimization has improved the fracture toughness of ceramic materials by 30±5% by carefully controlling the parameters of sintering. Using genetic algorithms, the thermal conductivity of alloys has been improved by 40-60% [104]. Experiments have shown that these predictions are accurate within 5% error margins.

AI-enhanced simulations demonstrate significant computational benefits. Molecular dynamics simulations that use machine learning potentials are 1000 times faster than regular Density functional theory (DFT) calculations and are 95% accurate in terms of quantum mechanics [64,65,73,82,101-104]. Neural networks speed up phase field modelling by reproducing microstructural evolution with a 92% correlation to experimental data and cutting computation time from weeks to hours [103]. Graph neural networks get R^2 scores of 0.94 for predicting bandgaps [104], which is 15% more accurate than traditional DFT [105].

Using AI in manufacturing has led to measurable improvements in production. Real-time control systems in additive manufacturing have cut dimensional errors by 75% and scrap rates from 12% to 3% [104]. Using predictive maintenance algorithms has added 40% more life to equipment and cut down on unplanned downtime by 65%. Quality control systems using computer vision detect micro-defects with 99.5% accuracy [64,65,73,82,101-104], improving product reliability by 30% compared to manual inspection.

Table 4. Quantitative performance metrics of ai applications in materials science

Application Domain	AI Technique	Key Metric	Ref
Materials Discovery	Neural Networks	Screening throughput	[2]
Property Prediction	Gradient Boosting	Prediction accuracy	[106]

Process Optimization	Bayesian Optimization	Yield improvement	[107]
Quality Control	Computer Vision	Defect detection	[56]
Simulation	ML Potentials	Computational speed	[17]
REE Leaching Optimization	XGBoost	Prediction error	[34]
REE Recovery	Ensemble ML	Recovery efficiency	

A quantitative result attained by different artificial intelligence methods used in materials science is shown in Table 4. All things considered, the findings demonstrate that AI significantly improves every phase of the materials development cycle, from quality assurance to discovery.

Neural networks allow for a remarkable acceleration of screening in the field of materials discovery, increasing the analysis speed by a factor of 100. This enhancement is especially beneficial for high-throughput research strategies and has been validated experimentally on 200 samples, adding to the approach's credibility. Gradient Boosting techniques provide high accuracy for property prediction; rigorous 10-fold cross-validation yielded a coefficient of determination of $R^2 = 0.92 \pm 0.03$. These findings show a dependable capacity to model complex systems.

10. CONCLUSION

The incorporation of Artificial Intelligence (AI) in material science has demonstrated a transformative impact, expediting progress in the discovery, optimization, and production of materials. This thorough review shows how AI methods like machine learning, neural networks, and genetic algorithms are changing the way materials are invented. AI-driven approaches have a lot of potential, as shown by their use in finding new materials, improving their properties, and making manufacturing processes better.

Even though there has been a lot of progress, there are still problems that need to be solved, such as making data easier to get to, making computations easier to understand, and making models easier to understand. Also, future developments need to take ethics into account. Still, the future of AI in material science looks bright, with new trends and collaborations between different fields opening the door to more breakthroughs.

As the field grows, AI will stay at the front, giving researchers and professionals powerful tools to open up new possibilities and push material science to new heights.

Author contributions:

Bendaoud Mebarek: Conceptualization, Methodology, Writing- Original Draft, Visualization,

Project administration, Supervision.

Joan-Josep Suñol: Conceptualization, Writing-Review & Editing, Supervision.

Mohamed Amine Daoud: Formal analysis, Writing-Original Draft, Visualization.

Yassine El Guerri: Methodology, Writing-Review & Editing, Visualization.

Abdelkader Alem: Validation, Resources, Writing-Review & Editing.

Mourad Keddami: Review & Editing, Supervision.

Conflicts of interest or competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The authors gratefully acknowledge the members of the Research Laboratory in Artificial Intelligence and Systems (LRIAS) at Ibn Khaldoun University.

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IZVOD

EVOLUIRAJUĆA ULOGA VEŠTAČKE INTELIGENCIJE U NAUCI O MATERIJALIMA: OD OTKRIĆA VOĐENIH PODACIMA DO BUDUĆIH IZGLEDA

Uključivanje veštačke inteligencije (VI) u nauku o materijalima pokrenulo je transformativnu promenu, olakšavajući značajan napredak u otkrivanju, optimizaciji i proizvodnji novih materijala. Ovaj pregled pruža sveobuhvatan pregled nedavnih razvoja, upotrebe i problema koji dolaze sa korišćenjem VI u ovoj oblasti. Razmatra najsavremenije metode poput mašinskog učenja, neuronskih mreža i genetskih algoritama i kako one mogu pomoći u ubrzanju razvoja novih materijala. Glavne oblasti upotrebe, kao što su pronalaženje novih materijala, poboljšanje svojstava postojećih, modeliranje i simulacija i poboljšanje proizvodnih procesa, detaljno su razmotrene. Iako je postignut veliki napredak, još uvek postoji mnogo problema koje treba rešiti, posebno kada je u pitanju kvalitet i dostupnost podataka, računaska složenost, interpretabilnost modela i etika. Ovaj pregled uključuje studije slučaja kako bi se pokazalo kako metode vođene VI mogu biti korisne i efikasne u nauci o materijalima. Takođe ukazuje na nove trendove i buduće pravce, naglašavajući mogućnosti saradnje između različitih oblasti i nove istraživačke mogućnosti.

Ključne reči: Veštačka inteligencija, nauka o materijalima, mašinsko učenje, optimizacija i inovacije.

Pregledni rad

Rad primljen: 23.07.2026.

Rad korigovan: 25.07.2026.

Rad prihvaćen: 29.07.2026.

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