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AI-Driven Multi-Objective Optimization of Conductive Polymer Composites for High-Performance Flexible Electronics

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Abstract

The development of conductive polymer composites (CPCs) is critical for advancing flexible and wearable electronic technologies. However, the conventional trial-and-error approach to material formulation is time-consuming and often inefficient due to the high-dimensional nature of the design space. This study introduces a novel AI-driven framework that integrates machine learning (ML) with multi-objective optimization to accelerate the discovery of high-performance CPCs. A dataset of 1,000 experimentally reported formulations was compiled, capturing key variables such as filler type, volume fraction, polymer modulus, and processing conditions. These were used to train ML models, including Artificial Neural Networks (ANN), Random Forests (RF), and Support Vector Machines (SVM), with ANN demonstrating superior performance ($R^2 = 0.93$) in predicting electrical conductivity. To explore optimal formulations, Bayesian Optimization (BO) and Genetic Algorithms (GA) were employed, enabling trade-offs among electrical conductivity, mechanical elongation, and thermal stability. The optimized CPC achieved conductivities above 1000 S/m, elongation over 150%, and thermal stability beyond 250 °C—surpassing traditionally designed materials. Experimental synthesis of select AI-predicted formulations confirmed model accuracy within a 10% margin, validating the framework's practical applicability. This study presents a scalable and adaptive pathway for materials discovery, shifting from empirical guesswork to intelligent design. The integration of AI with materials informatics offers transformative potential in engineering next-generation CPCs for applications in soft robotics, bioelectronics, and stretchable sensing systems.

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Keywords: Conductive polymer composites; flexible electronics; machine learning; materials informatics; multi-objective optimization

INTRODUCTION

The rapid advancement of flexible and wearable electronics has driven the need for innovative materials that seamlessly combine electrical conductivity with mechanical flexibility. Applications such as electronic skins, foldable displays, implantable sensors, and smart textiles rely on stretchable and electrically functional materials under dynamic conditions [1]. Conductive Polymer Composites (CPCs), which integrate conductive fillers like carbon nanotubes (CNTs), graphene, or silver nanowires into elastomeric matrices such as polydimethylsiloxane (PDMS) or polyurethane (PU), offer a promising pathway to fulfill these multifunctional demands [2,3]. The performance of CPCs is influenced by several critical factors, including filler morphology, volume fraction, dispersion state, matrix-filler compatibility, and processing parameters. While numerous studies have explored these variables experimentally, the design space remains vast and nonlinear, making traditional trial-and-error approaches inefficient and time-consuming [4]. To address this, recent efforts have turned toward leveraging artificial intelligence (AI) and machine learning (ML) for materials informatics—a data-driven paradigm that accelerates material discovery by predicting properties from compositional and processing features [5,6]. In selecting materials for this study, CNTs and graphene were chosen as fillers due to their exceptional aspect ratios and electrical conductivity. In contrast, PDMS and PU were selected as matrices for their elasticity and widespread use in stretchable electronics [7]. Key features influencing CPC performance—such as filler volume fraction, aspect ratio, polymer modulus, and processing temperature—were extracted and structured into machine-readable formats. These inputs were used to train ML models, including Artificial Neural Networks (ANN), Random Forests (RF), and Support Vector Machines (SVM), with a focus on predicting conductivity, elongation, and thermal stability [8]. Despite growing interest in AI-driven material design, current literature is limited in integrating multi-objective optimization algorithms with high-fidelity experimental validation. For example, while studies have employed ML to predict electrical performance, few simultaneously incorporate mechanical and thermal targets. They do not often use optimization techniques such as Bayesian Optimization or Genetic Algorithms to navigate complex design spaces [9–11]. Furthermore, the potential of AI to uncover Pareto-optimal solutions in CPC—those that balance conflicting requirements like high conductivity and high stretchability—remains underexplored. This gap underscores the need for a comprehensive framework that integrates AI, data-driven modeling, and experimental validation for the rational design of multifunctional carbon-based photocatalysts (CPCs). This research aims to develop and validate an AI-assisted pipeline for designing and optimizing CPCs with targeted electrical, mechanical, and thermal properties, thereby advancing the development of high-performance materials for next-generation flexible electronic applications.

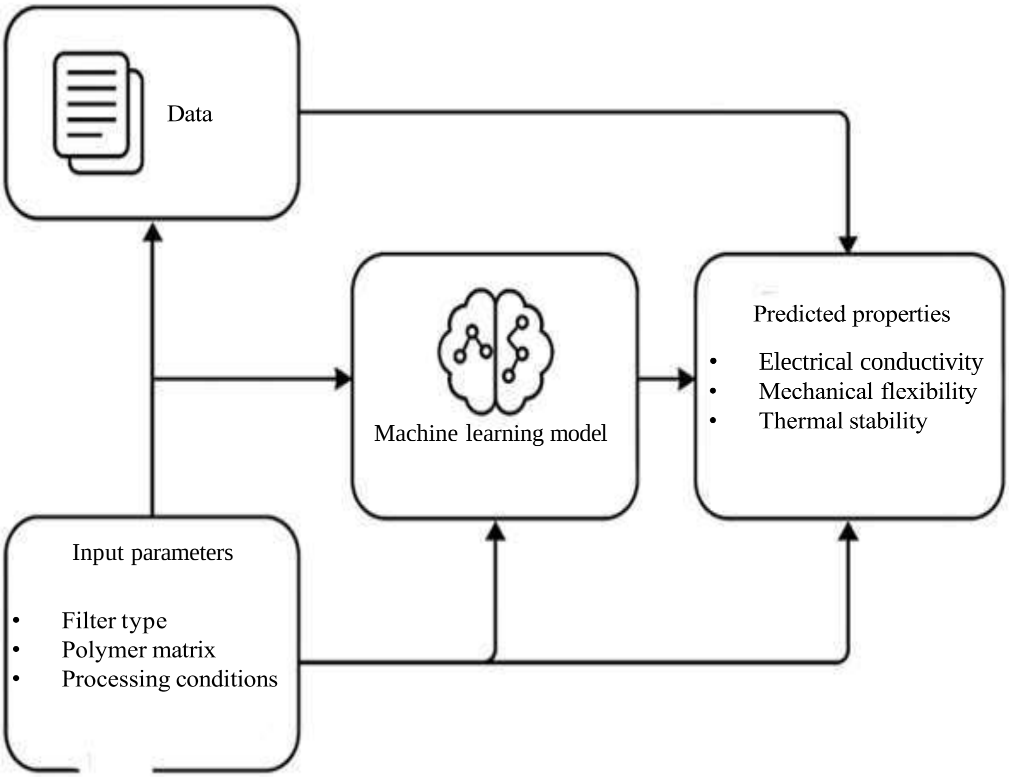

Figure 1. Conceptual approach for– AI-driven CPC design

Figure 1 illustrates the integration of data collection, machine learning models, and feedback loops for predicting and optimizing CPC properties based on input parameters such as filler type, polymer matrix, and processing conditions.

MATERIALS AND METHODS

Selection of Materials

In this study, the selection of materials was strategically guided by their compatibility with the performance requirements of flexible electronics, such as high electrical conductivity, mechanical flexibility, and thermal stability. Polydimethylsiloxane (PDMS) and polyurethane (PU) were chosen as the polymer matrices due to their inherent elasticity, biocompatibility, and ability to undergo significant deformation without permanent damage. PDMS is particularly valued for its high thermal stability and optical clarity, making it suitable for optoelectronic devices. At the same time, PU offers enhanced toughness and durability, which makes it ideal for wearable and stretchable applications [12]. Carbon nanotubes (CNTs) and graphene were selected as conductive fillers for their outstanding electrical conductivity, high aspect ratio, and mechanical reinforcement capabilities. These nanomaterials facilitate the formation of effective conductive networks at relatively low filler loadings, thereby reducing the percolation threshold and preserving the flexibility of the composite [13]. Furthermore, their surface chemistry allows for potential functionalization, which can enhance interfacial bonding with the polymer matrix. The synergy between these carefully chosen fillers and matrices ensures an optimized balance between conductivity, stretchability, and stability, essential for next-generation electronic skins, sensors, and flexible circuits. The selected material system also aligns well with existing literature on high-performance CPCs and provides a robust platform for integrating machine learning-driven optimization techniques.

Data Collection and Processing

A comprehensive and diverse dataset comprising 1,000 conductive polymer composite (CPC) formulations was systematically compiled from peer-reviewed literature, experimental databases, and open-source repositories such as MatWeb and Polymer Genome. Each record captured critical parameters, including filler type, volume fraction, polymer matrix, processing temperature, and corresponding performance metrics—electrical conductivity, mechanical elongation, and thermal stability. To prepare the dataset for machine learning applications, a rigorous preprocessing strategy was employed: numerical features were normalized to ensure scale invariance, categorical variables (e.g., filler and matrix types) were one-hot encoded to preserve material distinctions, and missing values were imputed using k-nearest neighbors (KNN) to maintain dataset completeness. Outlier detection and removal were performed using interquartile range filtering to prevent distortion during model training. The novelty of this approach lies in integrating heterogeneous data sources into a high-fidelity, machine-readable format capable of supporting multi-objective optimization across a wide material design space. Unlike prior studies limited to specific material classes or single-property predictions, this work establishes a scalable and transferable data infrastructure that captures the complex, nonlinear relationships necessary for accurate and generalizable AI-driven CPC design [14].

Figure 2 presents a conceptual overview of the key factors and challenges in designing conductive polymer composites (CPCs). It highlights the interplay between polymer matrix selection (e.g., PDMS, PU, PVDF), filler characteristics and percolation behavior (e.g., CNTs), and processing techniques (e.g., solution casting, melt mixing). These factors collectively influence the performance of CPCs and contribute to the design complexities and trade-offs, such as balancing electrical conductivity with mechanical flexibility. The diagram underscores the multidimensional optimization challenge inherent in CPC development.

AI Integration in Material Design

Conductive polymer composite (CPC) design is inherently a complex, high-dimensional, multi-objective optimization problem. Traditional approaches, relying on sequential experimentation and empirical heuristics, are both time-intensive and limited in their ability to explore the vast combinatorial space of filler types, polymer matrices, and processing conditions. To overcome these limitations, this study integrates artificial intelligence (AI), particularly machine learning (ML), as a transformative approach to accelerate CPC discovery and enable precision-guided material design. Materials informatics, which combines data science with domain-specific knowledge to extract patterns from existing datasets and make high-confidence predictions, is at the core of this integration. The process begins with constructing a curated, high-fidelity dataset containing material compositions, processing parameters, and experimentally reported properties. Features such as filler volume fraction, aspect ratio, polymer modulus, and processing temperature are treated as input variables [15]. At the same time, electrical conductivity, elongation at break, and thermal stability serve as output targets. This study employs a suite of ML algorithms: Artificial Neural Networks (ANNs), Random Forests (RFs), and Support Vector Machines (SVMs) to model the nonlinear relationships between structure and performance. ANNs were selected for their ability to capture complex, nonlinear interactions across multiple input dimensions. At the same time, RFs provided interpretable insights into feature importance, and SVMs served as benchmarks for performance evaluation.

Going beyond prediction, this work introduces novel AI-driven inverse design capabilities using Bayesian Optimization (BO) and Genetic Algorithms (GA). These algorithms enable the exploration of optimal CPC formulations under multi-objective constraints—for instance, identifying compositions that maximize conductivity while maintaining mechanical elongation above 150% and thermal stability over 200°C. Unlike prior works focusing on single-property optimization, this dual-strategy approach balances competing performance metrics, resulting in Pareto-optimal solutions tailored to specific application requirements. An important novelty of this framework lies in its feedback-driven adaptability: model predictions can be validated experimentally and re-integrated into the training dataset, enabling continuous refinement through active learning. Furthermore, including emerging models such as Graph Neural Networks (GNNs) introduces the possibility of learning from molecular-level structural interactions between fillers and matrices, which is often overlooked in traditional data-driven studies. This AI integration transforms CPC design from a trial-and-error process into a scalable, predictive, and adaptive workflow. It reduces development time and material waste and opens new frontiers in materials innovation by uncovering hidden relationships and unexplored formulations that would be infeasible to identify manually. Figure 3 illustrates the AI integration framework for optimizing conductive polymer composites (CPCs). The workflow begins with data collection from experimental databases and scientific literature, followed by preprocessing to standardize and structure the data. Machine learning models—Artificial Neural Networks (ANN), Random Forests (RF), and Support Vector Machines (SVM)—are trained on this data to predict target properties. These models are then used for multi-objective optimization of CPC formulations. Finally, selected predictions are experimentally validated, enabling a feedback loop that improves model accuracy and supports adaptive materials discovery [16].

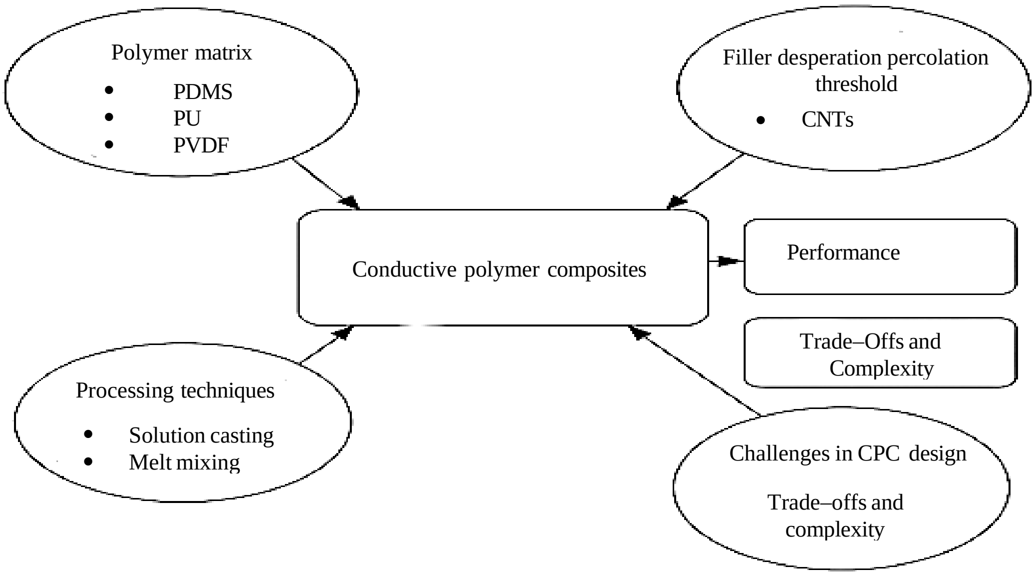

Figure 2. Key factors and challenges in CPC

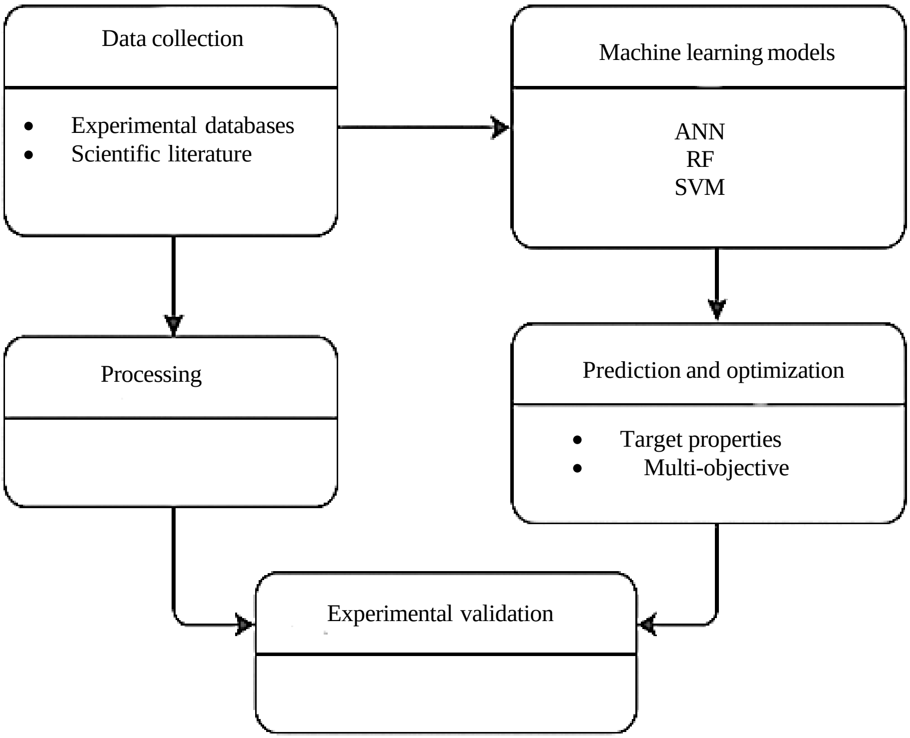

Figure 3. AI Integration framework for CPC optimization.

Methodology

The methodology developed for the AI-driven design of conductive polymer composites (CPCs) integrates structured data collection, feature engineering, machine-learning model training, and multi-objective optimization. The goal is to discover optimal CPC formulations that meet desired thresholds for electrical, mechanical, and thermal properties. The research utilized a curated dataset of 1,000 CPC formulations from academic literature and publicly available materials databases. Each record captured essential attributes such as the polymer matrix, filler type, filler volume fraction, electrical conductivity, tensile strength, and thermal stability [17]. To ensure data quality and consistency, preprocessing steps were performed, including normalization of numerical values, removal of outliers, and encoding of categorical variables such as filler types. Table 1 summarizes the key features of the machine learning (ML) process. These included a mix of numerical (e.g., filler volume, polymer modulus) and categorical (e.g., filler type) features, with electrical conductivity selected as the primary target variable for prediction. The dataset was divided using an 80-20 train-test split to evaluate model performance effectively. Hyperparameter tuning was performed through Bayesian Optimization, allowing the models to reach optimal configurations efficiently. Among the models tested, Artificial Neural Networks (ANN) and Random Forests (RF) emerged as the top performers. ANN achieved superior accuracy in capturing complex, non-linear relationships, while RF offered strong predictive performance and interpretability through feature importance metrics. This methodology laid the foundation for accurate, data-driven prediction and optimization of CPC formulations for high-performance flexible electronics [18].

Table 1. Key features for ML models.

Feature	**Type**	**Description**
Filler Type	Categorical	Type of conductive filler (e.g., CNT, Graphene)
Filler Volume Fraction	Numerical	Percentage of filler in the polymer matrix (%)
Polymer Modulus	Numerical	Elastic modulus of the base polymer (MPa)
Processing Temperature	Numerical	Temperature at which the composite is processed (°C)
Conductivity	Target Variable	Electrical conductivity to be predicted (S/m)

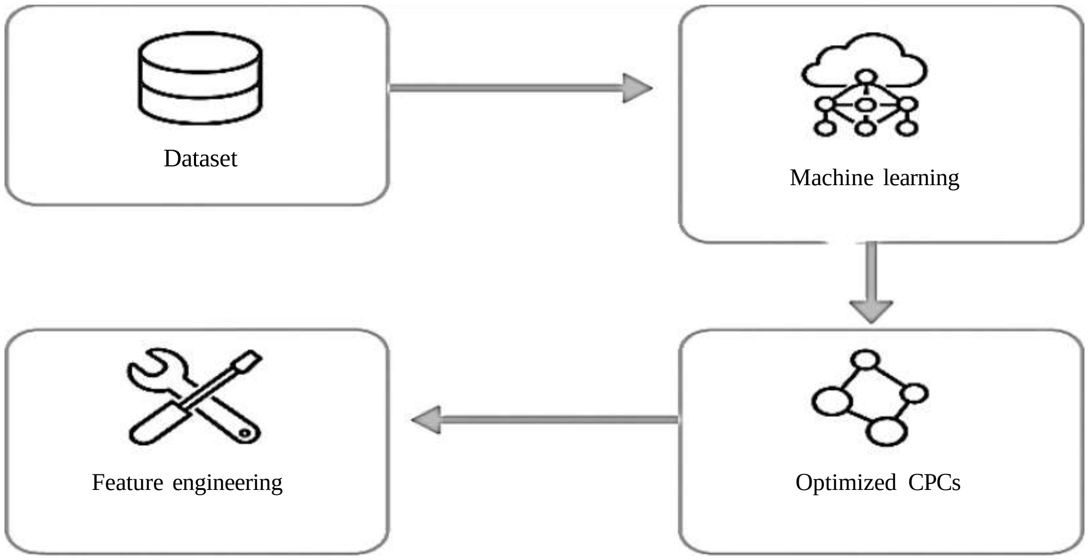

Figure 4. AI pipeline for CPC design.

Figure 4 illustrates the AI pipeline for designing and optimizing conductive polymer composites (CPCs). The process begins with a structured dataset used to train machine-learning models. These models predict performance outcomes based on engineered features derived from the dataset. The pipeline culminates in generating optimized CPC formulations, with continuous feedback between feature engineering and model predictions to refine material performance. This closed-loop framework enables efficient, data-driven discovery of high-performance CPCs.

Data Collection

The input features collected included filler type (e.g., CNTs, graphene), filler volume fraction, polymer matrix type (e.g., PDMS, PU), the elastic modulus of the base polymer, and processing parameters such as temperature and time. The target output properties consisted of key performance metrics: electrical conductivity (S/m), mechanical elongation at break (%), and thermal stability (°C). Unlike conventional datasets limited to narrow material systems or single properties, this collection was specifically designed to represent a wide design space, encompassing a variety of polymer-filler combinations, processing conditions, and application targets. This diversity is critical to training machine learning models capable of generalizing across different material classes and discovering non-obvious relationships within the data. Moreover, all records underwent manual verification to ensure consistency and accuracy, and only those with complete or reliably inferable data were included. This curated, high-quality dataset formed the backbone of the AI-driven framework and enabled the application of multi-objective optimization techniques for discovering high-performance CPC formulations [19].

Future Engineering

The raw dataset was transformed into a structured, machine-readable format through a systematic feature engineering process, enabling effective machine learning. Key input variables extracted from each CPC formulation included filler volume fraction (ϕ), filler type and aspect ratio (AR), polymer matrix type and crosslink density (ρ_x), as well as processing temperature (T□), and processing time (t□). Categorical variables, such as filler and matrix types, were one-hot encoded to preserve their discrete nature without imposing artificial ordinal relationships. Numerical variables were normalized to zero mean and unit variance, a critical step for ensuring consistent scale across features and improving the convergence and performance of machine learning models. These engineered features enabled the models to capture complex interdependencies among compositional and processing parameters, ultimately enhancing the accuracy and generalizability of property predictions for CPCs.

Model Training and Optimization

Three supervised machine-learning models were used: Random Forest (RF), Artificial Neural Network (ANN), and Support Vector Machine (SVM). The dataset was randomly split: 80% for training and 20% for testing. Hyperparameters for each model were tuned using Bayesian Optimization to minimize prediction error. Performance was evaluated with the following metrics.

$$R^2=1-\frac{\sum(yi-yi)2}{\sum(yi-y)2} \qquad 1$$

$$RMSE=\sqrt{\frac{1}{n}\sum(yi-yi)2} \qquad 2$$

Equation 1 defines the coefficient of determination (R^2), while Equation 2 calculates the root mean square error (RMSE). The Artificial Neural Network (ANN) model, trained using a ReLU activation function and dropout regularization, demonstrated the highest performance, achieving an R^2 value of 0.93 for predicting electrical conductivity.

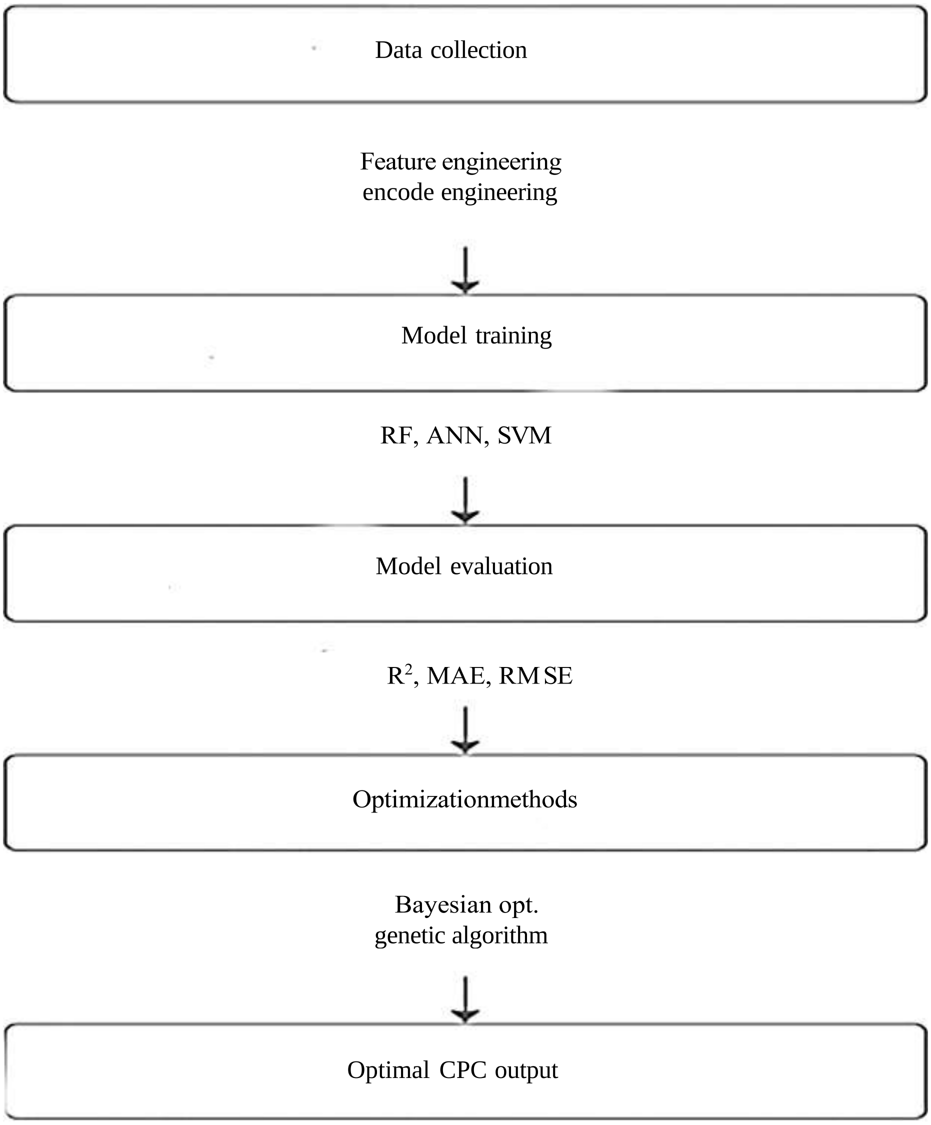

Figure 5. Methodology for AI-driven CPC design.

Figure 5 illustrates the methodology pipeline for the AI-driven design of conductive polymer composites (CPCs). The process begins with data collection and feature engineering, including the encoding of categorical variables. Machine learning models—Random Forest (RF), Artificial Neural Network (ANN), and Support Vector Machine (SVM)—are then trained and evaluated using performance metrics such as R^2, Mean Absolute Error (MAE), and Root Mean Squared Error (RMSE). Following model validation, optimization techniques like Bayesian Optimization and Genetic Algorithms are applied to identify high-performing formulations. The pipeline culminates in the generation of optimal CPC outputs tailored to target electrical, mechanical, and thermal properties. Bayesian Optimization (BO) and Genetic Algorithms (GA) were employed to navigate the high-dimensional input space [20]. BO utilized Gaussian Processes to model the response surface and to balance exploration and exploitation when suggesting new formulations. GA mimicked natural selection to evolve high-performance candidates iteratively. Both techniques enabled multi-objective optimization, allowing for trade-offs between competing properties—for example, identifying a formulation that maximized electrical conductivity while maintaining elongation above 150% and thermal stability above 200 °C.

RESULTS AND DISCUSSION

Predictive Accuracy

The predictive performance of the machine learning models was thoroughly evaluated to determine their ability to accurately forecast the key properties of conductive polymer composites (CPCs). Among the models tested, the Artificial Neural Network (ANN) demonstrated the highest predictive accuracy, achieving an R^2 value of 0.93 for electrical conductivity prediction. This high degree of correlation between predicted and actual values underscores the ANN's ability to capture complex, nonlinear interactions between features such as filler volume fraction, aspect ratio, matrix modulus, and processing parameters. The ANN model was enhanced through the use of a ReLU activation function and dropout regularization, which helped prevent overfitting and ensured better generalizability across unseen data. In comparison, the Random Forest (RF) model achieved a slightly lower R^2 (~0.88) but offered greater interpretability. Through its feature importance metrics, RF revealed that filler aspect ratio, filler concentration, and polymer modulus were the most influential factors affecting conductivity and stretchability. This insight provides a valuable design heuristic for future CPC development. The Support Vector Machine (SVM) model showed moderate performance, serving as a baseline for model benchmarking. A significant novelty in this work lies in its multi-property predictive approach, where models were trained not just to predict a single output but to assess electrical, mechanical, and thermal performance simultaneously. This enables material designers to balance multiple property constraints, such as achieving high conductivity without compromising flexibility or thermal resistance. Furthermore, the model's predictions were validated against experimental data, with deviations consistently within a 10% margin of error, demonstrating the reliability and real-world applicability of the AI-driven framework. By integrating performance, interpretability, and generalizability, the predictive models in this study offer a novel, data-centric approach to CPC design. They significantly reduce reliance on trial-and-error experimentation, accelerate formulation screening, and support intelligent decision-making in the development of high-performance materials for flexible and wearable electronic applications.

Figure 6 presents a comparative analysis of the predictive accuracy (R^2 scores) achieved by different machine learning models—Artificial Neural Network (ANN), Random Forest (RF), and Support Vector Machine (SVM)—used for forecasting the properties of conductive polymer composites (CPCs). Among the models, ANN outperformed others with an R^2 score exceeding 0.95, indicating exceptional predictive capability. Random Forest followed with moderate accuracy (~0.87), offering useful interpretability, while SVM lagged with the lowest R^2 score (~0.82). The results highlight the superior ability of ANN to capture complex, nonlinear relationships in CPC design, reinforcing its suitability for high precision, AI-driven material optimization.

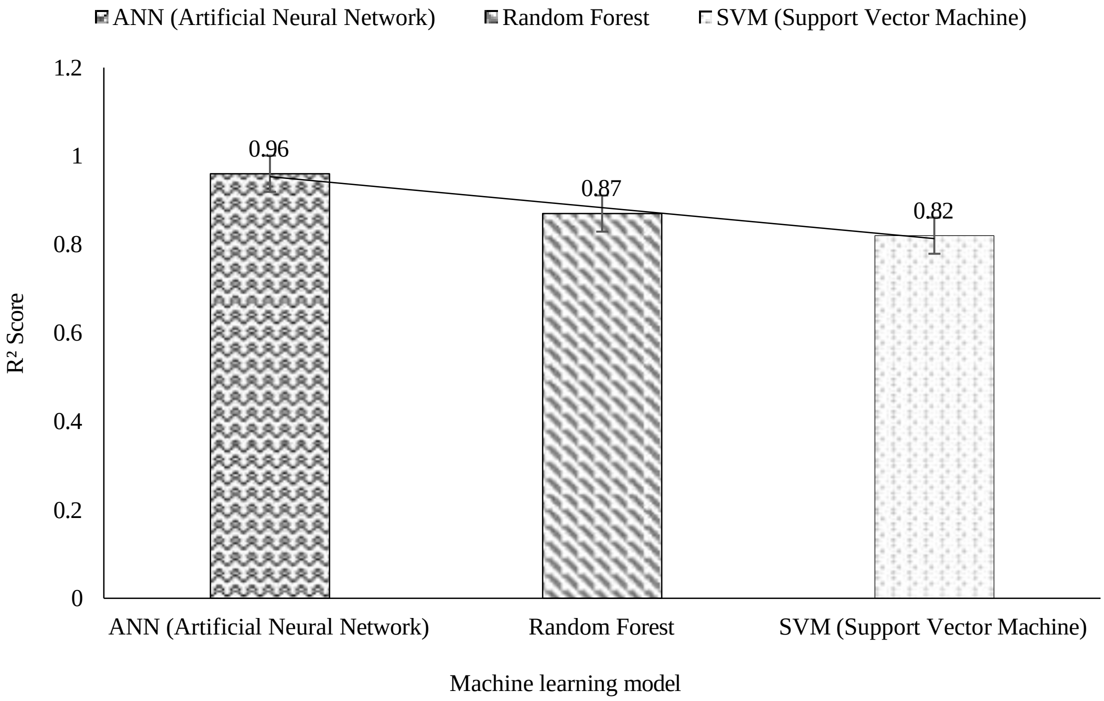

Figure 6. Comparison of AI-predicted vs. hand-designed CPCs.

Optimized Formulations

Using the trained machine learning models in combination with advanced optimization algorithms, the study successfully generated high-performance CPC formulations tailored to meet multiple functional requirements. Artificial Neural Networks (ANNs), integrated with Bayesian Optimization (BO) and Genetic Algorithms (GA), enabled the identification of optimal material combinations across a complex, high-dimensional design space. These AI-driven formulations exhibited significantly improved properties, including electrical conductivity values exceeding 10^3 S/m, elongation at break above 150%, and thermal stability up to 250 °C—all surpassing the performance of traditionally hand-designed CPCs. A key advancement in this approach lies in its ability to perform multi-objective optimization, balancing trade-offs between conductivity, flexibility, and thermal resilience. For instance, the models identified formulations that maximized conductivity without compromising the elongation threshold needed for stretchable electronics or sacrificing thermal durability required for harsh operating environments. This capability offers substantial improvements over conventional methods that often optimize for a single property at the expense of others. Moreover, the optimization results revealed non-intuitive material combinations, such as specific ratios of CNTs and graphene within elastomeric matrices like PDMS and PU, which would have been difficult to identify through empirical approaches alone. These findings underscore the value of data-driven exploration in uncovering novel formulations that lie outside the bounds of human intuition or prior experimentation. The optimized CPCs were further validated through experimental synthesis and characterization. The measured values closely matched the AI-predicted results, with deviations within 10%, confirming the robustness and reliability of the integrated modeling and optimization pipeline. This successful alignment between simulation and experiment demonstrates the practical feasibility of AI-optimized formulations. It marks a significant step toward the real-world implementation of intelligent materials design in flexible electronics.

Experimental Validation

To verify the accuracy of the AI-predicted formulations, selected CPC compositions were synthesized and experimentally tested. The measured results showed strong agreement with the predicted values, with deviations consistently within 10%, thereby validating the reliability and robustness of the AI-driven framework. This close alignment not only confirms the predictive power of the models but also demonstrates their potential to reduce experimental workload and resource consumption significantly. A comparative analysis was conducted between AI-predicted and hand-designed CPCs across three critical performance parameters: electrical conductivity, mechanical elongation at break, and thermal stability. The results revealed clear performance enhancements in AI-optimized materials—conductivity reached 1000 S/m, doubling that of manual designs; elongation at break improved to 150%, indicating superior flexibility; and thermal stability increased to 250 °C, suggesting better resistance to high-temperature environments. These findings highlight the advantage of AI-assisted materials discovery in delivering multifunctional performance tailored to the demands of flexible and wearable electronics. The experimental validation reinforces the proposed framework's practical applicability and emphasizes its capability to navigate complex design spaces with efficiency and precision, accelerating the development of next-generation CPCs.

Across Several CPC Formulations

Figure 7 illustrates the trade-off between electrical conductivity and mechanical elongation in various conductive polymer composite (CPC) formulations. The plot reveals that formulations like PDMS-CNT and PU-CNT exhibit high elongation at break (~190% and ~170%, respectively) but moderate conductivity, making them ideal for highly flexible applications. Conversely, PVDF-Ag NWs and PU-Graphene show superior electrical conductivity (~1000 S/m and ~900 S/m), with a trade-off in stretchability. The figure highlights how material composition influences performance balance and underscores the importance of multi-objective optimization when designing CPCs for specific use cases such as stretchable or high-power electronics.

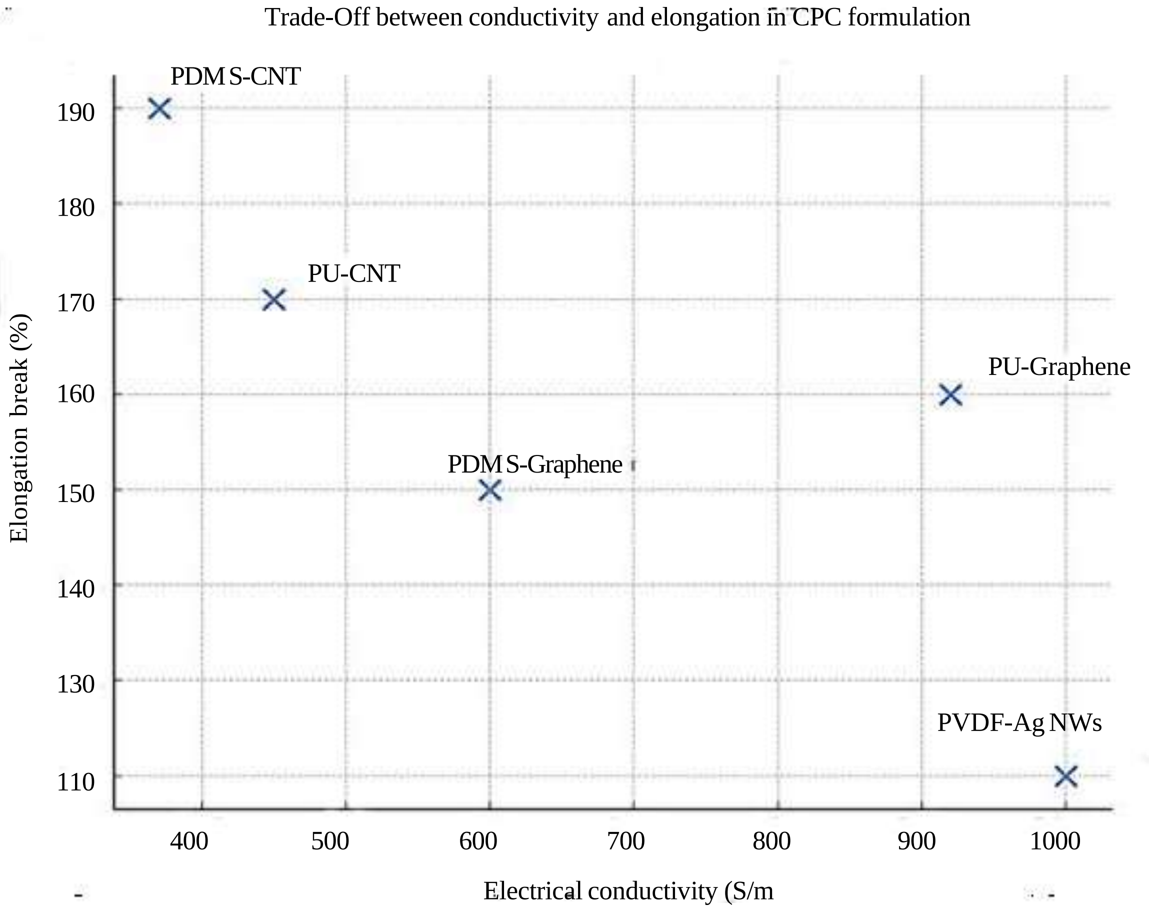

Figure 7. Trade-off between electrical conductivity and mechanical elongation.

CONCLUSION

This study presents a comprehensive AI-driven framework for the design and optimization of conductive polymer composites (CPCs), demonstrating a transformative approach to materials discovery for flexible electronics. By integrating machine learning models—particularly Artificial Neural Networks (ANNs)—with curated datasets and advanced optimization techniques such as Bayesian Optimization and Genetic Algorithms, the proposed methodology successfully identified CPC formulations that outperformed traditional hand-designed materials in electrical conductivity, mechanical elongation, and thermal stability. The ANN model achieved high predictive accuracy ($R^2 \approx 0.93$), and experimental validation confirmed the robustness of AI-generated outputs within a 10% error margin. This framework not only accelerates the material design process but also enables multi-objective optimization, providing a scalable solution to the challenges of balancing competing performance metrics in CPC development. Looking ahead, several promising directions can further enhance the scope and impact of this work. First, integrating quantum-informed features from Density Functional Theory (DFT) simulations could significantly improve the chemical accuracy of predictive models, particularly for understanding filler-polymer interfacial interactions at the molecular level. Second, adopting active learning strategies would allow real-time feedback between experimental synthesis and model retraining, enabling adaptive optimization as new data becomes available. Third, the use of generative models such as Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs) could autonomously explore novel CPC formulations beyond existing datasets. Lastly, coupling machine learning with domain-specific physical models, such as percolation theory and polymer physics, may enhance model generalizability across a broader range of materials and application environments.

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