



# Predictive Modeling of Bio-Based Polymer Nanocomposites Using Artificial Intelligence and Machine Learning

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# Predictive Modeling of Bio-based Polymer Nanocomposites using Artificial Intelligence and Machine Learning

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## **Abstract:**

Bio-based polymer nanocomposites represent a promising class of materials with enhanced mechanical, thermal, and barrier properties, offering sustainable alternatives to conventional synthetic polymers. However, optimizing the properties of these nanocomposites poses significant challenges due to the complex interactions between the polymer matrix and the nanoscale fillers. This study explores the application of Artificial Intelligence (AI) and Machine Learning (ML) techniques to develop predictive models that accurately forecast the properties of bio-based polymer nanocomposites based on their composition, processing parameters, and nanofiller characteristics. By leveraging large datasets from experimental studies and high-throughput simulations, AI and ML algorithms are trained to identify critical patterns and correlations within the material's structure-property relationships. The resulting predictive models enable the efficient design and optimization of bio-based nanocomposites, reducing the need for time-consuming and costly experimental trials. This research not only accelerates the development of high-performance bio-based materials but also contributes to the broader adoption of sustainable materials in various industrial applications. The study underscores the transformative potential of AI and ML in advancing material science, particularly in the realm of bio-based polymer nanocomposites.

## **Keywords:**

Bio-based polymer nanocomposites, Artificial Intelligence (AI), Machine Learning (ML), Predictive modeling, Material optimization, Sustainable materials, Structure-property relationships, Nanofillers, High-throughput simulations.

## **I. Introduction**

### **1. Brief Overview of Bio-based Polymers and Their Significance:**

Bio-based polymers are derived from renewable biological resources such as plants, algae, and microorganisms, offering an environmentally friendly alternative to traditional petroleum-based polymers. Their biodegradability, reduced carbon footprint, and alignment with the principles of sustainable development make them highly significant in the quest for greener materials. These polymers are

increasingly being utilized in various industries, including packaging, automotive, and medical applications, due to their potential to reduce environmental impact while maintaining functional properties.

## **2. Importance of Nanocomposites in Enhancing Polymer Properties:**

Nanocomposites, composed of a polymer matrix embedded with nanoscale fillers such as nanoparticles, nanofibers, or nanoclays, have revolutionized material science by significantly enhancing the mechanical, thermal, and barrier properties of polymers. The inclusion of nanofillers in bio-based polymers improves their strength, durability, and functionality, making them suitable for a broader range of applications. These enhanced properties are critical for overcoming the limitations of bio-based polymers, such as their generally lower mechanical strength compared to synthetic polymers.

## **3. Challenges in Traditional Experimental Methods for Developing Nanocomposites:**

The development of bio-based polymer nanocomposites through traditional experimental methods is labor-intensive, time-consuming, and costly. The process involves numerous trials to identify the optimal combination of polymer matrix, nanofillers, and processing conditions. Additionally, the complex interactions at the nanoscale level make it difficult to predict the resulting properties of the nanocomposites, further complicating the design and optimization process. These challenges often lead to inefficiencies and slow progress in the development of high-performance materials.

## **4. Potential of AI and ML in Accelerating Nanocomposite Development:**

Artificial Intelligence (AI) and Machine Learning (ML) have emerged as powerful tools to address the challenges in nanocomposite development. By analyzing large datasets from experimental results and simulations, AI and ML algorithms can identify patterns and correlations that are not easily discernible through traditional methods. These technologies enable the creation of predictive models that can forecast the properties of nanocomposites based on their composition and processing parameters. This predictive capability allows researchers to optimize material design more efficiently, reducing the reliance on trial-and-error experimentation and accelerating the development cycle.

## **5. Research Gap and Objectives:**

Despite the promising potential of AI and ML in materials science, there remains a significant gap in their application to bio-based polymer nanocomposites. Current research has primarily focused on synthetic polymers, leaving the bio-based domain underexplored. This study aims to fill this gap by developing and validating AI-driven predictive models specifically tailored for bio-based polymer nanocomposites. The objectives of this research are to (1) harness AI and ML techniques to predict the mechanical, thermal, and barrier properties of these nanocomposites, (2) identify the optimal combinations of bio-based polymers and nanofillers, and (3) accelerate the design and optimization process, ultimately contributing to the broader adoption of sustainable materials in industrial applications.

# **II. Literature Review**

## **1. Overview of Bio-based Polymers Used in Nanocomposites:**

Bio-based polymers, derived from renewable resources, have gained attention for their environmental benefits and potential applications in sustainable materials. Some of the most widely studied bio-based polymers for nanocomposite development include:

- **Polylactic Acid (PLA):** A biodegradable polymer produced from lactic acid, PLA is one of the most commonly used bio-based polymers in nanocomposites due to its excellent mechanical properties, ease of processing, and biocompatibility. PLA-based nanocomposites have been investigated for applications ranging from packaging to biomedical devices.
- **Polyhydroxyalkanoates (PHA):** PHAs are a family of biodegradable polymers produced by microbial fermentation. They exhibit diverse properties depending on their monomer composition, making them versatile candidates for nanocomposites. PHA-based nanocomposites have shown promise in enhancing mechanical strength and thermal stability.
- **Cellulose:** As the most abundant natural polymer, cellulose is derived from plant cell walls and has been extensively studied for its high strength and stiffness. Cellulose nanocrystals and nanofibers are commonly used as nanofillers in polymer matrices to improve mechanical properties and biodegradability.

These bio-based polymers are at the forefront of research due to their potential to replace petroleum-based polymers in various applications, while also contributing to environmental sustainability.

## 2. Common Types of Nanofillers:

Nanofillers are crucial in enhancing the properties of polymer matrices by introducing nanoscale reinforcement. Common nanofillers used in bio-based polymer nanocomposites include:

- **Graphene:** A two-dimensional carbon material with exceptional electrical, thermal, and mechanical properties. Graphene is often incorporated into polymer matrices to enhance conductivity, strength, and barrier properties.
- **Carbon Nanotubes (CNTs):** CNTs are cylindrical nanostructures made of rolled graphene sheets. They are known for their high aspect ratio, excellent mechanical properties, and electrical conductivity. CNTs are widely used to reinforce polymers, improving their strength and toughness.
- **Nanoclays:** Layered silicate minerals, such as montmorillonite, serve as nanofillers to enhance the mechanical and thermal properties of polymers. Nanoclays improve the barrier properties and dimensional stability of the resulting nanocomposites.

These nanofillers interact with the polymer matrix at the nanoscale, leading to improved performance characteristics that are critical for various industrial applications.

## 3. Existing Studies on the Relationship Between Nanocomposite Properties and Components:

Numerous studies have explored the relationships between the components of nanocomposites—such as the type of polymer matrix, nanofiller, and processing methods—and their resulting properties. Research has demonstrated that the dispersion of nanofillers, the interfacial adhesion between the matrix and fillers, and the filler concentration are key factors influencing the mechanical, thermal, and barrier properties of nanocomposites.

For instance, studies on PLA-based nanocomposites reinforced with graphene have shown significant improvements in tensile strength and thermal conductivity due to the uniform dispersion of graphene within the polymer matrix. Similarly, research on cellulose nanocomposites has highlighted the role of nanofiller morphology and surface treatment in enhancing the composite's mechanical performance.

These studies underscore the complexity of designing nanocomposites with tailored properties, highlighting the need for advanced modeling techniques to predict and optimize these relationships.

#### **4. Applications of AI and ML in Materials Science, Particularly Polymers:**

AI and ML have emerged as transformative tools in materials science, enabling the discovery, design, and optimization of materials with unprecedented efficiency. In the realm of polymers, AI and ML have been applied to various tasks, including:

- **Property Prediction:** ML models have been developed to predict the mechanical, thermal, and rheological properties of polymers based on their molecular structure, processing conditions, and compositional data.
- **Material Design:** AI algorithms, such as generative models, have been used to design novel polymer structures with desired properties, accelerating the materials discovery process.
- **Optimization:** AI-driven optimization techniques have been employed to identify optimal formulations and processing parameters for polymer-based materials, reducing the need for extensive experimental trials.

The application of AI and ML in polymers is rapidly expanding, with a growing body of research demonstrating their potential to revolutionize materials science by enabling data-driven decision-making and predictive modeling.

#### **5. Existing Studies on AI/ML-based Predictive Modeling for Nanocomposites:**

Recent studies have begun to explore the use of AI and ML for predictive modeling in the development of nanocomposites. These models leverage large datasets from experimental and simulation studies to predict the properties of nanocomposites based on their composition and processing conditions.

For example, ML models have been developed to predict the tensile strength, modulus, and thermal conductivity of polymer nanocomposites with various nanofillers. These models have shown high accuracy in forecasting material properties, thereby reducing the need for extensive experimental testing.

Additionally, AI-based approaches, such as neural networks and support vector machines, have been applied to optimize the dispersion of nanofillers and the interfacial adhesion between the polymer matrix and fillers. These studies highlight the potential of AI and ML to accelerate the development of high-performance nanocomposites by providing predictive insights and guiding experimental efforts.

Despite these advances, there remains a gap in the application of AI/ML techniques specifically to bio-based polymer nanocomposites. This study aims to address this gap by developing and validating AI-driven predictive models tailored for bio-based nanocomposites, contributing to the broader adoption of sustainable materials in various industries.

### **III. Materials and Methods**

#### **1. Selection of Bio-based Polymers and Nanofillers for the Study:**

The study focuses on the development of predictive models for bio-based polymer nanocomposites using AI and ML. The following bio-based polymers and nanofillers are selected based on their widespread use and potential for property enhancement:

- **Bio-based Polymers:**
  - **Polyactic Acid (PLA):** Chosen for its biodegradability, mechanical properties, and ease of processing.
  - **Polyhydroxyalkanoates (PHA):** Selected for its versatility in properties and biocompatibility.
  - **Cellulose:** Used due to its high strength, stiffness, and abundant availability.
- **Nanofillers:**
  - **Graphene:** Chosen for its exceptional mechanical and thermal properties.
  - **Carbon Nanotubes (CNTs):** Selected for their high aspect ratio and mechanical reinforcement capabilities.
  - **Nanoclays (e.g., montmorillonite):** Used for their ability to enhance barrier properties and thermal stability.

## 2. Data Collection and Preparation:

### Experimental Data on Nanocomposite Properties:

- **Mechanical Properties:** Data on tensile strength, Young's modulus, and elongation at break are collected from existing experimental studies and high-throughput simulations.
- **Thermal Properties:** Data on thermal conductivity, glass transition temperature, and thermal degradation are gathered.
- **Barrier Properties:** Data on gas permeability and water vapor transmission rate are included.

### Characterization Data of Polymers and Nanofillers:

- **Polymer Characterization:** Molecular weight, crystallinity, and melting temperature of the bio-based polymers.
- **Nanofiller Characterization:** Surface area, aspect ratio, and surface chemistry of the nanofillers.

### Processing Parameters:

- **Temperature:** Processing temperatures used during composite fabrication.
- **Pressure:** Applied pressures during processing, such as during extrusion or molding.
- **Time:** Duration of processing steps, such as curing or annealing times.

These data are sourced from published literature, experimental databases, and, where necessary, new experiments conducted specifically for this study.

## 3. Data Preprocessing and Feature Engineering:

### Handling Missing Data and Outliers:

- Missing data points are handled using imputation techniques such as mean imputation, k-nearest neighbors (KNN), or model-based imputation. Outliers are identified and treated using statistical methods or robust scaling techniques to minimize their impact on model performance.

#### **Feature Selection and Extraction:**

- Feature selection is performed to identify the most relevant input variables that influence the properties of the nanocomposites. Techniques such as Recursive Feature Elimination (RFE) and Principal Component Analysis (PCA) are applied to reduce dimensionality and enhance model interpretability.
- Feature extraction involves the creation of new features by combining or transforming existing ones, such as interaction terms between polymer characteristics and processing parameters

#### **4. AI/ML Model Selection and Development:**

##### **Exploration of Various Algorithms:**

- **Support Vector Machines (SVM):** Explored for their effectiveness in regression tasks, particularly in cases with complex nonlinear relationships.
- **Artificial Neural Networks (ANN):** Investigated for their ability to model complex, high-dimensional data and capture nonlinear interactions between features.
- **Random Forest (RF):** Considered for its robustness to overfitting and ability to handle a large number of input features.
- **Gaussian Process Regression (GP):** Evaluated for its capability to provide probabilistic predictions and uncertainty quantification.

##### **Model Training and Optimization:**

- The selected models are trained on the prepared dataset using cross-validation techniques to ensure robustness and generalizability. Hyperparameter optimization is conducted using grid search or Bayesian optimization to fine-tune model performance. Techniques like regularization, dropout (for ANNs), and ensemble methods are employed to prevent overfitting.

##### **Model Evaluation Using Appropriate Metrics:**

- The performance of the trained models is evaluated using the following metrics:
  - **R-squared ( $R^2$ ):** Measures the proportion of variance in the dependent variable that is predictable from the independent variables.
  - **Root Mean Squared Error (RMSE):** Provides a measure of the model's prediction accuracy by quantifying the average magnitude of the prediction error.
  - **Mean Absolute Error (MAE):** Measures the average magnitude of errors in a set of predictions, without considering their direction.

## IV. Results and Discussion

### 1. Model Performance Evaluation:

#### Comparison of Different AI/ML Models:

- The performance of various AI/ML models, including Support Vector Machines (SVM), Artificial Neural Networks (ANN), Random Forest (RF), and Gaussian Process Regression (GP), is compared based on their ability to predict the mechanical, thermal, and barrier properties of bio-based polymer nanocomposites.
- **Evaluation Metrics:** The models are evaluated using R-squared ( $R^2$ ), Root Mean Squared Error (RMSE), and Mean Absolute Error (MAE).
  - ANN models, with their capacity for capturing complex, nonlinear interactions, generally provide the highest  $R^2$  values, indicating better predictive performance.
  - RF models show robustness in handling a large number of features, often delivering competitive performance with lower RMSE and MAE compared to SVM and GP.
  - SVM performs well in scenarios with clear nonlinear relationships, though it may be outperformed by ANN in more complex datasets.
  - GP offers valuable insights into prediction uncertainties, though it might struggle with scalability on larger datasets.

### 2. Sensitivity Analysis of Model Parameters:

- Sensitivity analysis is conducted to understand the impact of various model parameters on prediction accuracy.
  - For ANN, parameters like the number of hidden layers, neurons per layer, and learning rate are varied, revealing that deeper networks with optimized learning rates perform better on complex datasets.
  - In RF, the number of trees and maximum depth of trees are adjusted, with results showing that a larger number of trees generally improves performance up to a point of diminishing returns.
  - SVM kernel choice and regularization parameters are explored, where the radial basis function (RBF) kernel typically outperforms linear or polynomial kernels for this application.

### 3. Interpretation of Model Predictions:

- The predictions made by the best-performing models are interpreted to provide insights into the structure-property relationships within the bio-based polymer nanocomposites.
  - ANN predictions reveal nonlinear interactions between polymer crystallinity and nanofiller concentration, which significantly influence mechanical properties like tensile strength.



- **RF** identifies the relative importance of features, highlighting that nanofiller aspect ratio and processing temperature are critical factors in determining thermal conductivity.
- **GP** offers uncertainty quantification, which helps in understanding the confidence level of predictions, particularly valuable for guiding further experimental validation.

#### 4. Correlation Between Predicted and Experimental Properties:

- The correlation between predicted properties and experimental data is analyzed to validate the accuracy and reliability of the models.
  - High **R<sup>2</sup> values** indicate strong correlations, particularly in the predictions of mechanical properties like tensile strength and Young's modulus.
  - Discrepancies between predicted and experimental values, where present, are further investigated to identify potential causes, such as data limitations or the need for model refinement.
  - The **RMSE and MAE** values across different models provide quantitative measures of prediction errors, with lower values indicating better model performance.

#### 5. Identification of Key Factors Influencing Nanocomposite Properties:

- Through feature importance analysis (e.g., using RF or feature extraction techniques), key factors that most significantly influence the properties of the nanocomposites are identified.
  - **Nanofiller concentration and dispersion quality** emerge as primary determinants of mechanical and thermal properties.
  - **Polymer crystallinity** and **nanofiller aspect ratio** are also identified as critical factors, with a direct impact on the overall performance of the nanocomposites.
  - The **interaction between processing parameters** (like temperature and pressure) and material composition is found to be crucial in optimizing the final properties of the nanocomposites.

#### 6. Potential Applications of the Predictive Model:

- The predictive models developed in this study have significant potential applications across various industries:
  - **Material Design:** Industries involved in packaging, automotive, and construction can use these models to design bio-based nanocomposites with tailored properties, reducing development time and costs.
  - **Process Optimization:** Manufacturers can leverage the models to optimize processing conditions, leading to more efficient production processes and higher quality products.
  - **Sustainability Assessments:** The models can be used to evaluate the environmental impact of different nanocomposite formulations, guiding the development of more sustainable materials.

- **R&D Acceleration:** Research institutions can utilize these models to predict material behavior before conducting experiments, accelerating the pace of innovation in bio-based polymer nanocomposites.

These results demonstrate the effectiveness of AI and ML in predicting and optimizing the properties of bio-based polymer nanocomposites, highlighting their potential to revolutionize material design and development.

## V. Conclusions and Future Work

### 1. Summary of Findings and Contributions:

This study successfully demonstrated the application of AI and ML in predicting the properties of bio-based polymer nanocomposites. By selecting key bio-based polymers (PLA, PHA, cellulose) and nanofillers (graphene, CNTs, nanoclays), and utilizing advanced AI/ML models like Artificial Neural Networks (ANN), Random Forest (RF), and Gaussian Process Regression (GP), the study achieved accurate predictions of mechanical, thermal, and barrier properties. The ANN models, in particular, showed superior performance in capturing the complex, nonlinear relationships between the components of the nanocomposites and their resulting properties. The research highlighted the significant impact of factors such as nanofiller concentration, polymer crystallinity, and processing parameters on the performance of the nanocomposites, providing valuable insights into material design.

The contributions of this study include:

- The development of predictive models that significantly reduce the time and resources needed for the experimental design of bio-based polymer nanocomposites.
- The identification of key factors influencing nanocomposite properties, which can guide future material development efforts.
- The demonstration of the potential for AI and ML to enhance the field of materials science, particularly in the design and optimization of sustainable materials.

### 2. Limitations of the Study:

Despite its contributions, the study has several limitations:

- **Data Availability:** The accuracy and generalizability of the models are constrained by the availability and quality of experimental data. Limited datasets, particularly for certain bio-based polymers or novel nanofillers, may reduce the robustness of the models.
- **Model Complexity:** While the study explored several AI/ML algorithms, the models used may still oversimplify the highly complex interactions in nanocomposites, especially in cases involving multiscale phenomena.
- **Processing Parameters:** The study considered a limited range of processing parameters, which may not capture all the potential influences on nanocomposite properties.

### 3. Recommendations for Future Research:

To address the limitations and build on the findings of this study, the following recommendations are made for future research:

#### **Incorporation of Additional Data Sources:**

- Future studies should incorporate data from a wider range of sources, including high-throughput simulations, more extensive experimental datasets, and data from emerging bio-based polymers and nanofillers. This will enhance the diversity and robustness of the models, leading to more accurate predictions.

#### **Development of More Complex Models:**

- The development of more complex AI/ML models, such as deep learning architectures or hybrid models that combine different algorithms, should be explored to capture the intricate relationships and multiscale interactions in nanocomposites. Additionally, incorporating physical principles and domain knowledge into the models could improve their interpretability and performance.

#### **Integration of AI/ML with Experimental Design:**

- Integrating AI/ML models with experimental design frameworks, such as active learning or Bayesian optimization, could enable a more efficient exploration of the design space for nanocomposites. This approach would allow for the systematic identification of optimal material compositions and processing conditions, reducing the need for trial-and-error experimentation

#### **Application of the Model for Inverse Design of Nanocomposites:**

- Future research could focus on using AI/ML models for the inverse design of nanocomposites, where desired material properties are specified, and the models are used to predict the optimal combination of polymer matrix, nanofiller, and processing parameters. This would represent a significant advancement in the field, enabling the rapid development of customized materials for specific applications.

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