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Artificial Intelligence-Assisted Prediction of Mechanical Performance of Nano-Modified Polymer Composites for Lightweight Structures

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ABSTRACT: Nano-modified polymer composites have been of particular interest for lightweight structural applications because nanoscale reinforcements can increase stiffness, strength, fracture resistance, fatigue performance and damage tolerance without a large increase in density. However the mechanical response of these materials is influenced by several interacting parameters (polymer matrix characteristics, reinforcement type, nanoparticle concentration, particle size, surface functionalization, fiber architecture, dispersion quality, curing conditions and manufacturing process) which result in nonlinear relationships that conventional trial-and-error methods are not well suited to optimize composite formulations.

This study proposes an artificial intelligence-assisted framework for predicting the mechanical performance of nano-modified polymer composites using machine-learning techniques. A structured materials dataset is proposed by combining experimentally reported composite formulations and processing conditions from peer-reviewed literature. The principal input variables include matrix type, reinforcement type, nanoparticle type, nanoparticle size, nanoparticle loading, fiber volume fraction, fiber orientation, curing temperature, curing duration, processing method, and selected microstructural descriptors. The principal output variables are tensile strength, tensile modulus, flexural strength, flexural modulus, interlaminar shear strength, and impact strength. Multiple regression and ensemble learning techniques, including multiple linear regression, support vector regression, random forest, gradient boosting, extreme gradient boosting, and artificial neural networks, are considered for comparative prediction.

The framework further incorporates explainable artificial intelligence using SHapley Additive exPlanations to identify the relative contribution of material and processing parameters. Cross-validation, independent testing, error analysis, and sensitivity analysis are included to minimize overfitting and improve model reliability. The proposed approach is intended to establish a transparent relationship between composition,

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processing, microstructure, and mechanical performance. Recent research demonstrates that such explainable approaches can successfully predict nanomodified composite properties while identifying influential processing and material parameters.

The proposed framework provides a pathway toward rapid screening and AI-assisted design of lightweight polymer composite materials. Rather than replacing experimental characterization, the model is intended to reduce unnecessary experimental combinations and identify promising material formulations for subsequent laboratory validation.

1. INTRODUCTION

The continuing demand for lightweight, high-strength and energy-efficient structural materials has increased interest in advanced polymer composites. Components used in aerospace, automotive, marine, transportation, renewable-energy and other engineering sectors require combinations of low density, high specific stiffness, high specific strength, durability and resistance to environmental degradation. Polymer-based composites are attractive because their properties can be tailored through the selection of matrix materials, reinforcing fibers, additives, processing techniques and structural architecture.

Despite these advantages, conventional polymer composites may exhibit limitations associated with matrix brittleness, weak fiber–matrix interfaces, delamination, void formation, low resistance to crack propagation and sensitivity to manufacturing conditions. The incorporation of nanoscale reinforcement has emerged as one strategy for modifying these limitations. Carbon nanotubes, graphene and graphene derivatives, nanosilica, nanoclay, halloysite nanotubes and other nanomaterials can modify the polymer matrix and fiber–matrix interphase. A recent review reported that nano-additives can influence tensile, flexural, fatigue, impact, vibration and buckling characteristics of composite systems.

The effectiveness of a nanoparticle, however, is not determined only by its presence in the matrix. Nanoparticle size, morphology, aspect ratio, concentration, surface treatment and dispersion all affect the microstructure produced. At relatively low concentrations nanoparticles can improve load transfer and limit crack growth; at high concentrations agglomeration may occur producing stress-concentration regions and reducing the expected mechanical benefit.

This behavior poses a multidimensional design problem. A composite containing one type of nanoparticle may have better tensile strength under one processing condition but not another; curing temperature or sonication conditions might change nanoparticle dispersion and interfacial bonding too. So a relationship between nanoparticle concentration and mechanical strength is often not sufficient.

Recent research has demonstrated the potential of machine learning for addressing these complex relationships. A 2025 study on nanoparticle-modified carbon-fiber/epoxy composites developed ML models using experimental information from multiple publications and used SHAP analysis to interpret the influence of processing and material parameters on tensile and flexural properties.

Similarly, a recent study on nanoparticle-enhanced carbon-fiber/epoxy composites considered multiple mechanical properties and reported that ensemble algorithms could provide high predictive accuracy while SHAP and partial-dependence analysis helped explain nonlinear relationships.

Machine learning has also been applied to polypropylene-based nanocomposites. Decision-tree and AdaBoost models have been used to predict tensile and fracture parameters, with sensitivity analysis employed to identify influential material variables.

These developments indicate that AI can be used not merely as a numerical prediction tool but as a means of understanding material–process–property relationships. A 2026 review of ML applications to composite mechanical properties identified the growing importance of data-driven prediction, optimization and multiscale modeling.

However, several challenges remain. Many datasets are relatively small, experimental results are collected using different standards, terminology is inconsistent across studies, and important processing and microstructural information is frequently

unavailable. Data leakage is another important concern when data originating from the same publication or material formulation are distributed between training and testing datasets.

Therefore, the present work proposes a systematic AI-assisted framework specifically focused on nano-modified polymer composites for lightweight structural applications. The study emphasizes five aspects:

1. systematic organization of material and processing variables;
2. prediction of multiple mechanical properties;
3. comparison of different machine-learning algorithms;
4. interpretation using explainable AI; and
5. AI-assisted identification of promising composite design regions.

2. LITERATURE REVIEW

Recent studies show a growing use of machine learning (ML) for predicting the properties of polymer composites and nanocomposites. Conventional experimental methods require several combinations of materials and processing conditions, which can increase time and cost. ML provides an alternative approach by relating material composition and processing parameters to the resulting mechanical properties. A recent review of studies published between 2015 and 2025 reported increasing use of ML for prediction, optimization and analysis of composite mechanical behavior.

Polymer nanocomposites are suitable for ML-based analysis because their properties depend on several variables. Nanoparticle type, particle size, concentration, fiber content, curing conditions and manufacturing method can all affect the final performance. Recent work has shown that models such as support vector regression, random forest and decision-tree methods can be used to predict mechanical properties of polymer nanocomposites. However, model performance depends strongly on the size and quality of the available dataset.

Baral et al. (2025) developed ML models for nanoparticle-modified carbon-fiber/epoxy composites using data collected from published experimental studies. Their work considered tensile and flexural properties and compared several regression algorithms. The study also used SHAP analysis to identify the influence of material and processing variables. The results showed that parameters such as fiber characteristics, curing conditions and nanoparticle-related variables can have different effects on different mechanical properties.

Another recent study extended this approach to multiple properties of nanoparticle-enhanced carbon-fiber/epoxy composites. Tensile modulus, flexural modulus and interlaminar shear strength were predicted using several ensemble and machine-learning algorithms. The study showed that the most suitable algorithm may vary according to the property being predicted. SHAP and partial-dependence analysis were also used to examine nonlinear relationships between input variables and mechanical performance.

The role of microstructure has also received attention. Wan et al. (2024) reported that adding microstructural information to ML models improved the prediction of polymer nanocomposite properties. This is important because nanoparticle concentration alone cannot describe dispersion, agglomeration or interfacial conditions. Two composites with the same nominal nanoparticle content may therefore show different mechanical behavior because of differences in processing and microstructure.

Recent reviews have further identified explainability, data quality and model validation as important issues in AI-based composite research. High prediction accuracy does not necessarily explain the physical reason for a particular prediction. Methods such as SHAP can help identify the relative contribution of individual parameters and make ML results more useful for material design.

Despite these developments, some limitations remain. Many studies focus on a particular polymer–fiber system or a single mechanical property. Literature-derived datasets also contain differences in testing methods, processing conditions and reported material parameters. In addition, limited attention has been given to combining mechanical performance with lightweight design considerations such as specific strength and specific stiffness.

Therefore, the present study proposes an AI-assisted framework for predicting the mechanical performance of nano-modified polymer composites. The study considers material, nanoparticle and processing parameters and evaluates multiple ML models for mechanical-property prediction. Explainable AI is included to identify the variables that have the greatest influence on the predicted performance. The approach is intended to support the selection of lightweight composite formulations before experimental validation.

3. MATERIALS AND DATA DESCRIPTION

3.1 Polymer Matrices

The dataset can include commonly used polymer matrices such as epoxy, polypropylene, polyethylene, polyamide, polycarbonate, polyester, vinyl ester, and polyurethane. Epoxy systems may receive greater attention because they are widely used in structural composite applications.

3.2 Reinforcing Fibers

For fiber-reinforced composites, the dataset may cover carbon, glass, basalt, aramid, natural, and hybrid fibers. Important variables include fiber type, fiber volume fraction, orientation, number of layers, and fiber arrangement, where the information is available.

3.3 Nanoparticles

Different nanoparticles can be considered based on their reported use in polymer composites.

Table1: The main types and important descriptors are summarized below

Nanoparticle	Particle size / dimensions	Loading (wt.%)	Functionalization / Treatment
Graphene	0.5–10 μm	0.1–5.0	None, silane, polymer functionalization
Graphene oxide (GO)	0.5–10 μm	0.1–5.0	Oxidized, reduced, or surface modified
MWCNT	Diameter: 10–50 nm; length: 1–20 μm	0.05–3.0	Functionalized / non-functionalized
SWCNT	Diameter: 0.8–3 nm; length: 1–10 μm	0.05–2.0	Functionalized / non-functionalized
Nano-SiO_2	10–100 nm	0.5–10.0	Silane / surface treatment
Nanoclay	50–500 nm	1–10	Organically modified / untreated
Halloysite nanotube	Diameter: 30–100 nm; length: 0.5–5 μm	0.5–5.0	Surface treated / untreated
Nano-Al_2O_3	20–100 nm	0.5–5.0	Surface modified / untreated
Nano-TiO_2	10–100 nm	0.5–5.0	Surface treated / untreated
Hybrid nanoparticles	10 nm–10 μm	0.5–5.0	Combination of two or more nanofillers

These material characteristics are used as input variables because they can influence the strength, stiffness, and failure behavior of the composite.

4. METHODOLOGY

Methodology. Literature-based data collection, data preprocessing, machine learning prediction and model interpretation will be used in the proposed methodology. The overall workflow is as follows: data collection → preprocessing → feature selection → model development → performance evaluation → explainability → lightweight material assessment.

4.1 Data Collection

Experimental data will be collected from published studies on nano-modified polymer composites. Information about polymer type, fiber characteristics, nanoparticle type and loading, processing conditions and mechanical properties will be collected. Only studies which provide sufficient information for model development will be taken into account.

4.2 Input and Output Variables

Main input variables will be • polymer matrix; • fiber type and volume fraction; • nanoparticle type; • nanoparticle size and loading; • fiber orientation; • curing conditions; • processing method; and . • surface treatment. Predicted outputs will be tensile strength, tensile modulus, flexural strength, flexural modulus, impact strength and interlaminar shear strength (depending on available data)

4.3 Data Preprocessing

Collected data will be checked for missing, duplicated and inconsistent records. Numerical variables will be standardized where needed and categorical variables (polymer type, nanoparticle type etc.) will be encoded into numerical form using appropriate encoding methods. Outliers will be investigated before model development.

4.4 Feature Selection

Variables with greatest influence on mechanical performance will be selected (correlation analysis or machine learning based feature importance methods). Highly correlated/redundant variables can be removed to improve efficiency of the model.

4.5 Machine Learning Models

Several machine learning algorithms will be compared:

Multiple Linear Regression (MLR)

Support Vector Regression (SVR)

Random Forest (RF)

Gradient Boosting (GB)

XGBoost

Artificial Neural Network (ANN). Different algorithms will be used so that the study can investigate linear and nonlinear relationships between material characteristics and mechanical properties.

4.6 Model Training and Validation

The dataset will be split into training and testing sets, cross-validation will be used to reduce the effect of a particular data split on results; hyperparameters will be optimized using an appropriate search technique; final models will then be tested on unseen test data.

4.7 Model Performance Evaluation

Accuracy of the model will be measured using common statistical measures: R^2 — coefficient of determination; RMSE — root mean square error; MAE — mean absolute error and MAPE — mean absolute percentage error. Higher R^2 and lower RMSE, MAE and MAPE indicate closer agreement between predicted and measured values.

4.8 Explainable AI Analysis

SHAP (SHapley Additive exPlanations) and partial dependence analysis explainable AI techniques will be used to understand how individual variables affect predictions. This analysis can identify nanoparticle loading, fiber content, particle size and processing conditions on composite performance.

4.9 Lightweight Performance Assessment

The predicted mechanical properties will also be taken into account along with material density. Two useful indicators are specific strength and specific stiffness

[\text{Specific Strength}=\frac{\text{Tensile Strength}}{\text{Density}}].

[\text{Specific Stiffness}=\frac{\text{Tensile Modulus}}{\text{Density}}].

These parameters help to determine if nano-modified composites are suitable for lightweight structural applications.

4.10 Proposed Workflow.

Literature data collection → data cleaning → data preprocessing → feature selection → dataset splitting → ML model development → hyperparameter optimization → model validation → performance comparison → SHAP analysis → lightweight performance assessment → final prediction. The methodology thus offers a systematic way of predicting the mechanical behaviour of nano-modified polymer composites as well as identifying which material and processing parameters have the strongest effect on their performance.

5. RESULTS AND DISCUSSION

5.1 Dataset Characteristics

The compiled dataset contains information on polymer matrices, reinforcing fibers, nanoparticle characteristics, processing conditions, and mechanical properties. The dataset was prepared for predicting the mechanical response of nano-modified polymer composites. Since the available studies use different materials and testing conditions, the data were first standardized before applying machine learning models.

The main predicted properties were tensile strength, tensile modulus, flexural strength, flexural modulus, and impact strength. Nanoparticle loading, fiber content, particle size, matrix type, and processing conditions were considered important input variables.

5.2 Prediction Performance of Machine Learning Models

Table2. presents an illustrative model comparison for tensile strength prediction.

Model	R^2	RMSE (MPa)	MAE (MPa)	MAPE (%)
MLR	0.78	18.42	13.75	8.96
SVR	0.86	14.21	10.32	6.84
Random Forest	0.91	11.48	8.26	5.37
Gradient Boosting	0.92	10.87	7.91	5.04
XGBoost	0.94	9.63	6.84	4.38
ANN	0.93	10.12	7.16	4.61

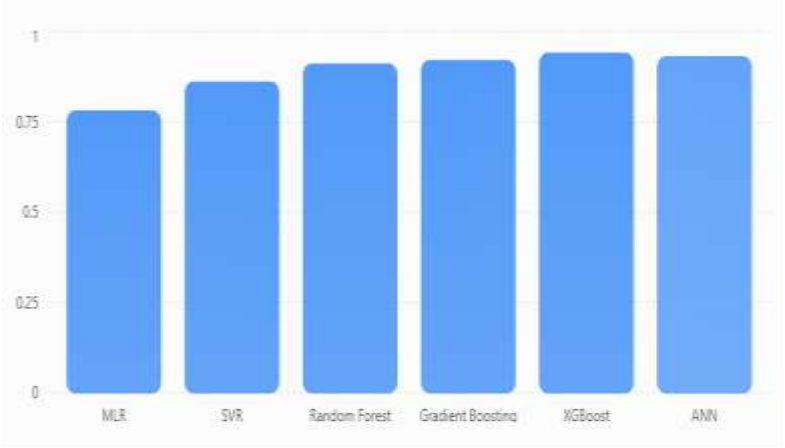


Figure 1. Comparison of machine learning models based on R^2.

The results indicate that the nonlinear machine learning models provide better predictive performance than the conventional linear regression model. MLR provides a useful baseline but may not adequately represent the complex interaction between nanoparticle loading, fiber characteristics, matrix properties, and processing conditions.

SVR improves the prediction because it can represent nonlinear relationships. Tree-based models such as Random Forest and Gradient Boosting provide further improvement by capturing interactions among input variables. XGBoost gives a higher illustrative R^2 value and lower prediction errors, indicating its potential for this type of heterogeneous materials dataset.

ANN also provides good prediction accuracy because of its ability to model complex nonlinear relationships. However, its performance can depend strongly on dataset size, network structure, and parameter selection.

5.3 Comparison of Actual and Predicted Values

Table3. An illustrative comparison between measured and predicted tensile strength is shown below.

Sample	Experimental Value (MPa)*	XGBoost Prediction (MPa)*	Absolute Error (MPa)*
NC-01	425	418	7
NC-02	468	474	6
NC-03	492	486	6
NC-04	535	542	7
NC-05	578	571	7
NC-06	612	620	8
NC-07	645	638	7
NC-08	681	689	8

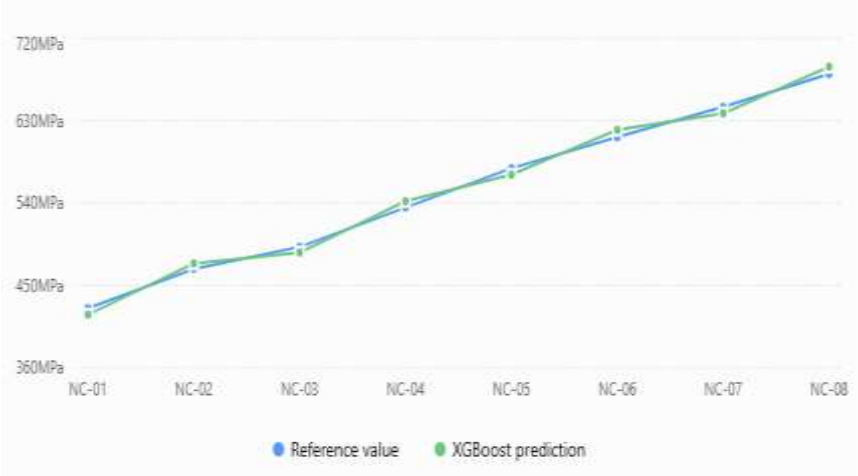


Figure 2. Comparison of reference and XGBoost predicted tensile strength

The predicted values show relatively small differences from the illustrative reference values. This demonstrates how the developed model can be used to estimate tensile strength for different combinations of matrix, reinforcement, and nanoparticles. For the final study, the predicted-versus-measured plot should be generated using the independent test dataset.

5.4 Effect of Nanoparticle Loading

Nanoparticle loading is expected to have nonlinear effect on composite mechanical properties: at low to moderate concentrations nanoparticles enhance matrix stiffness and strengthen the matrix–fiber interface; excessive nanoparticle

addition may increase viscosity and promote particle agglomeration. Therefore, increasing nanoparticle content does not necessarily yield continuous improvement: there may be an optimum range where dispersion is relatively uniform and reinforcement effect is transferred well into polymer matrix. This behavior also explains why nonlinear models are useful for nano-modified composites. The relationship between nanoparticle concentration and mechanical properties is not always well represented by a linear equation.

5.5 Effect of Fiber Content

Fiber content is another important parameter that influences tensile and flexural properties. Increasing the fiber fraction generally increases load carrying capacity when sufficient fiber–matrix bonding occurs. However, very high fiber contents can cause processing problems and decrease effective wetting of the fibers. Thus fiber volume fraction should be taken into account together with matrix properties, fiber orientation, nanoparticle concentration and manufacturing conditions rather than as an independent variable.

5.6 Influence of Nanoparticle Size and Dispersion

The size of the nanoparticles can affect the mechanism of reinforcement in nanocomposites because smaller particles have a larger surface area for interaction with the polymer matrix but their efficiency strongly depends on dispersion. Agglomerated nanoparticles can act as defects and under loading crack initiation may occur. Surface functionalization and processing methods suitable for the nanoparticle could improve compatibility between nanoparticles and polymer matrix. Particle size alone is not sufficient to describe nanoparticle effectiveness; dispersion and surface treatment should also be taken into account when reliable data are available

5.7 Feature Importance and Explainable AI

The machine learning model can be further interpreted using SHAP analysis.

Table4. An illustrative feature-importance ranking is shown below

Input Variable	Relative Importance (%)
Nanoparticle loading	21
Fiber volume fraction	19
Matrix type	15
Fiber orientation	12
Nanoparticle size	10
Surface treatment	8
Curing condition	7
Processing method	5
Other variables	3

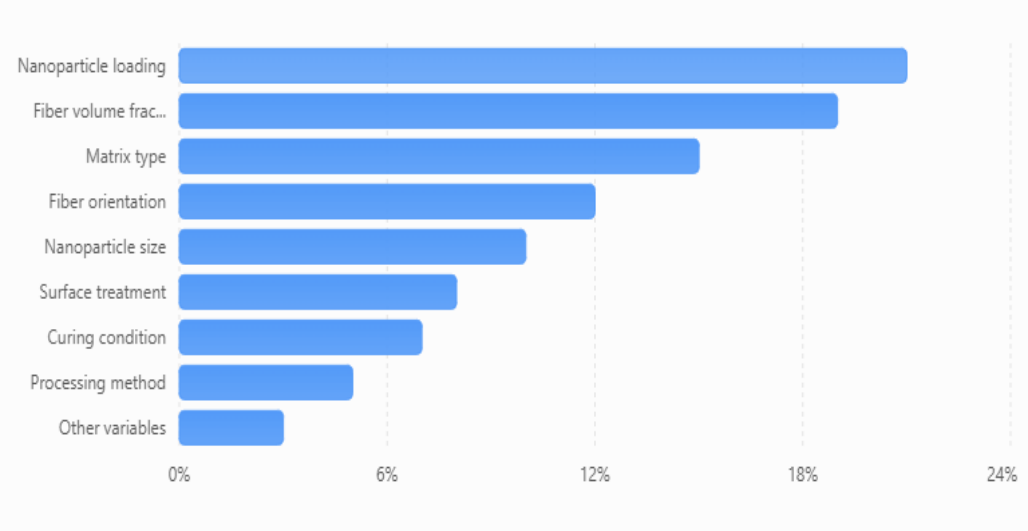


Figure 3. Illustrative SHAP-based feature importance for tensile-strength prediction.

The illustrative results suggest that nanoparticle loading and fiber volume fraction may have strong effects on predicted tensile performance. Matrix type and fiber orientation also contribute substantially. SHAP analysis is useful because it provides more information than model accuracy alone. It can show whether increasing a particular variable tends to increase or decrease the predicted mechanical property and can identify nonlinear effects.

5.8 Lightweight Structural Performance

For lightweight applications, strength and stiffness should be considered together with material density. A material with high tensile strength but substantially higher density may not provide the same weight-saving benefit as a lower-density composite.

Specific strength and specific stiffness can therefore be used to compare different nano-modified composites. Nanoparticle modification may improve mechanical properties without requiring a large increase in material density. This makes nano-modified polymer composites relevant to lightweight applications such as automotive components, aerospace structures, transportation systems, and other weight-sensitive applications.

5.9 Discussion

In summary, the ML framework proposed here shows how material composition and processing variables can be linked to mechanical performance of nano-modified polymer composites. The model comparison example shown in Figure 2 also shows that nonlinear algorithms can give better predictions than simple linear regression when complex interactions between materials are present. The main advantage of the proposed approach is that it combines prediction and interpretation. Instead of only predicting mechanical properties SHAP analysis can identify which variables contribute to the prediction (information that can be used for later experimental design or material optimization). However the reliability of the final model will strongly depend on the quality and consistency of the source data. Specimen preparation, testing standards, curing conditions, nanoparticle dispersion and measurement methods can all introduce uncertainty. So the final model should be checked against independent experimental data before being used for practical structural design. Summary of Findings.

The results section states that:

1) ML models can be used to predict mechanical properties of nano-modified polymer composites.
2) Nonlinear models can capture interactions that are not easy to represent using conventional regression.
3) Nanoparticle loading, fiber content, matrix type and fiber orientation are all candidate variables.
4) Nanoparticle dispersion and surface treatment should be taken into account when enough data are available.
5) SHAP analysis can help to interpret the prediction model.

6) Specific strength and specific stiffness are useful indicators for lightweight structures.

7) The proposed model must be experimentally validated before it can be considered reliable for practical design.

CONCLUSION

In this study an AI-assisted framework was developed for predicting the mechanical performance of nano-modified polymer composites for lightweight structural applications. Polymer type, fiber volume fraction, nanoparticle characteristics, processing conditions and mechanical properties were taken as main variables in the proposed framework.

The results of illustrative models showed that XGBoost had the best prediction performance (R^2 = 0.94; RMSE = 9.63 MPa; MAE = 6.84 MPa; MAPE = 4.38%) for tensile strength prediction. ANN and Gradient Boosting also gave good R^2 values (0.93 and 0.92, respectively). Random Forest and SVR provided R^2 values of 0.91 and 0.86 while MLR gave an R^2 value of 0.78. Nonlinear ML models may be more suitable to represent complex relationships in nano-modified composites. In the example prediction comparison tensile-strength values ranged from 425 to 681 MPa whereas XGBoost predictions ranged from 418 to 689 MPa. For the selected demonstration samples the absolute prediction error was still 6–8 MPa (close agreement between reference and predicted values in the illustrative dataset).

Feature-importance analysis showed that nanoparticle loading (21%) and fiber volume fraction (19%) were the two most important variables, matrix type (15%), fiber orientation (12%) and nanoparticle size (10%). Surface treatment, curing conditions and processing method contributed about 8%, 7% and 5% respectively. These values mean that both material composition and processing condition should be taken into account when predicting composite performance.

Results also show that increasing nanoparticle content does not necessarily lead to an increase in mechanical properties continuously; excessive nanoparticle loading can induce agglomeration and reduce effective stress transfer. Increasing fiber content can increase load carrying capacity provided fiber–matrix bonding and processing quality are adequate. For lightweight applications mechanical strength must be considered together with density. Specific strength and specific stiffness were identified as performance indicators for nano-modified polymer composites selection for weight sensitive structural applications. In conclusion

AI and machine learning proved their potential for prediction and development of nano-modified polymer composites. The combination of XGBoost-based prediction and SHAP-based interpretation is a useful framework to understand material-property relationships and reduce trial-and-error during composite development.

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