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EXPLAINABLE MACHINE LEARNING ANALYSIS OF ELECTRICAL CONDUCTIVITY IN GRAPHENE–POLYMER COMPOSITES

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Abstract

Electrical conductivity in graphene–polymer composites varies over many orders of magnitude because conductive pathways form only when graphene flakes become sufficiently connected. This study analyzes a literature-derived dataset of 486 graphene–polymer composite samples using Random Forest and Gradient Boosting models. The input descriptors were polymer matrix, filler type, processing route, system classification, and graphene loading. The conductivity target was expressed as $\log_{10}(\sigma)$ to reduce its wide dynamic range. On the fixed test split, Gradient Boosting achieved the best performance, with R^2=0.91, RMSE=1.36, and MAE=0.93 in $\log_{10}(\sigma)$ space, compared with R^2=0.84, RMSE=1.77 and MAE=1.45 for Random Forest. The results indicate that graphene loading alone does not explain conductivity variation across heterogeneous systems. Grouped feature-importance analysis showed that graphene loading (34.1%), system classification (32.6%), and processing route (20.8%) had the largest relative contributions to the model predictions, whereas polymer matrix (9.1%) and filler type (3.2%) showed lower grouped importance. These percentages represent model-based relative importance rather than causal physical contributions. Microstructural descriptors, including graphene aspect ratio, dispersion quality, and agglomeration state, were not consistently reported in the source literature and therefore, they were not included among the five model inputs; their absence remains an important source of predictive uncertainty. Overall, interpretable machine learning provides a useful framework for analysing conductivity trends in literature-derived datasets while making explicit the limitations of the available data.

Keywords: *Electrical percolation, Electrical conductivity, Explainable machine learning, Gradient Boosting, Graphene–polymer composites, Random Forest.*

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PHÂN TÍCH ĐỘ DẪN ĐIỆN CỦA COMPOSITE GRAPHENE–POLYMER BẰNG HỌC MÁY CÓ KHẢ NĂNG DIỄN GIẢI

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Tóm tắt

Độ dẫn điện của composite graphene–polymer biến thiên qua nhiều bậc độ lớn do các đường dẫn điện chỉ hình thành khi các tấm graphene đạt mức độ liên kết đủ lớn trong nền polymer. Nghiên cứu này phân tích bộ dữ liệu gồm 486 mẫu composite graphene–polymer được tổng hợp từ các công bố khoa học bằng hai mô hình Random Forest và Gradient Boosting. Năm biến đầu vào được sử dụng gồm polymer nền, loại chất độn, quy trình chế tạo, nhóm hệ vật liệu và hàm lượng graphene. Biến mục tiêu được biểu diễn dưới dạng $\log_{10}(\sigma)$ nhằm giảm ảnh hưởng của khoảng biến thiên rất rộng của biến mục tiêu. Trên tập kiểm tra cố định, mô hình Gradient Boosting cho kết quả tốt nhất với R^2=0.91, RMSE=1,36 và MAE=0.93 trong không gian $\log_{10}(\sigma)$ so với R^2=0.84, RMSE=1,77 và MAE=1,45 của mô hình Random Forest. Kết quả cho thấy riêng hàm lượng graphene không đủ để giải thích sự biến thiên độ dẫn điện giữa các hệ vật liệu không đồng nhất. Phân tích độ quan trọng theo nhóm biến cho thấy hàm lượng graphene (34,1%), nhóm hệ vật liệu (32,6%) và quy trình chế tạo (20,8%) có mức độ quan trọng tương đối cao nhất đối với kết quả dự đoán, trong khi polymer nền (9,1%) và loại chất độn (3,2%) có mức độ quan trọng thấp hơn. Các tỷ lệ phần trăm này biểu thị độ quan trọng tương đối dựa trên mô hình, không phải tỷ lệ đóng góp nhân quả vào độ dẫn điện. Các thông tin vi cấu trúc như tỷ lệ hình dạng, chất lượng phân tán và trạng thái kết tụ của graphene không được báo cáo nhất quán trong các công bố nguồn nên không được đưa vào năm biến đầu vào của mô hình; sự thiếu vắng các thông tin này vẫn là một nguồn bất định quan trọng của kết quả dự đoán. Nhìn chung, học máy có khả năng diễn giải cung cấp một khuôn khổ hữu ích để phân tích xu hướng độ dẫn điện từ dữ liệu công bố, đồng thời làm rõ những hạn chế của dữ liệu hiện có.

Từ khóa: *Composite graphene–polymer, Độ dẫn điện, Gradient Boosting, Học máy có khả năng diễn giải, Random Forest, Thấm điện.*

1. Introduction

Graphene–polymer composites have been widely studied because small amounts of graphene can strongly change the electrical conductivity of an insulating polymer matrix (Kim et al., 2010; Kuilla et al., 2010). This behavior is usually explained by electrical percolation. When the graphene content approaches a critical level, isolated flakes begin to form connected pathways, and the conductivity may be increased by several orders of magnitude (Sahimi, 1996; Stauffer & Aharony, 1992). However, the reported percolation threshold varies considerably among studies, from very low filler contents to several wt%, depending on graphene morphology, reduction state, aggregation, polymer matrix, and processing route (He & Tjong, 2013; Zare et al., 2024). Recent reviews also show that the processing method can be as important as graphene loading because it affects dispersion, flake contact, and network formation (Tarhini & Tehrani-Bagha, 2023).

Classical percolation theory is useful for interpreting the sharp conductivity increase in a single composite system, but it is less straightforward to apply to literature-derived datasets that combine different polymers, fillers, fabrication methods, and measurement conditions (Sahimi, 1996; Stauffer & Aharony, 1992). Even at similar graphene loadings, reported conductivities can differ substantially owing to variations in matrix chemistry, filler quality, dispersion state, and interflake contact (He & Tjong, 2013; Zare et al., 2024). Machine-learning methods have recently been used to predict composite properties and handle nonlinear relationships that are difficult to describe using simple empirical equations (Milad et al., 2022; Gupta et al., 2026; Raza et al., 2025). Nevertheless, many studies still focus mainly on prediction accuracy, while the relative influence of processing route, polymer matrix, filler type, and graphene loading on electrical percolation remains less clearly discussed.

In this work, we analyze a literature-derived dataset of 486 graphene–polymer composite samples using Random Forest and Gradient Boosting models. The conductivity is modeled as $\log_{10}(\sigma)$ because the reported values span more than seventeen orders of magnitude. The objectives are to evaluate the ability of tree-based models to predict electrical conductivity and to interpret the grouped feature importance in relation to conductive-network formation. By combining prediction metrics with physically informed interpretation, the study aims to clarify how material descriptors and processing-related factors contribute to conductivity variation across heterogeneous graphene–polymer composite systems.

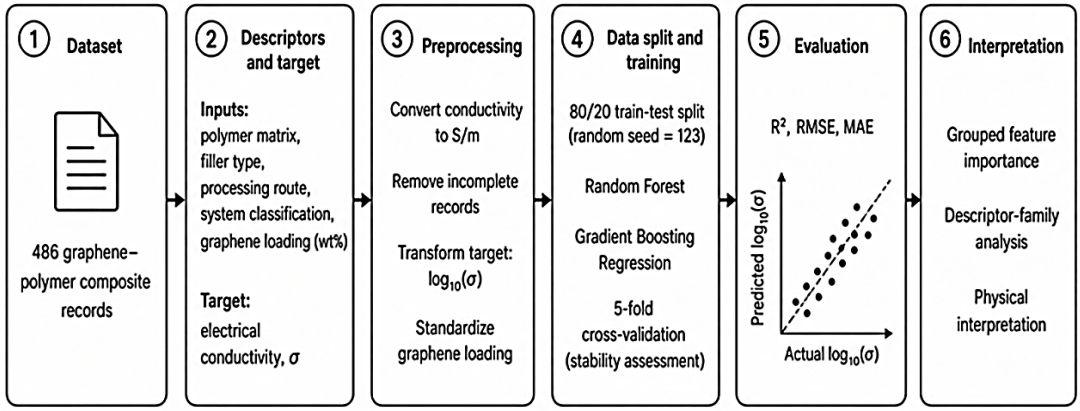

Figure 1. Machine-learning workflow used for dataset compilation, descriptor selection, data preprocessing, model training and validation, performance evaluation, and grouped feature-importance analysis.

Figure 1 summarizes the machine-learning workflow used in this study, including dataset compilation, descriptor selection, data preprocessing, model training and validation, performance evaluation, and grouped feature-importance analysis.

2. Dataset and preprocessing

2.1. Dataset composition

The dataset compiled for this study contains 486 graphene–polymer composite records from peer-reviewed publications reporting electrical conductivity. The records cover a range of polymer matrices, graphene-based fillers, fabrication methods, and composite-system classifications. For each record, the following information was retained when available: electrical conductivity, graphene loading, polymer matrix, filler type, processing route, and system classification.

Five variables were used as model inputs: polymer matrix, filler type, processing route, system classification, and graphene loading (wt%). Electrical conductivity was used as the prediction target. Because the records originated from independent publications, all conductivity values were converted to the SI unit of S/m before analysis (Kuilla et al., 2010). Records without the target value or any of the five required input descriptors were excluded from model training, leaving 258 complete records for machine-learning analysis.

Temperature was not used as an input descriptor because most reported measurements were performed near room temperature, providing limited variability for model development (Sun et al., 2022; Zare et al., 2024). In addition, several microstructural descriptors known to affect electrical transport, such as graphene aspect ratio, lateral size distribution, reduction degree, dispersion quality, orientation, and agglomeration state, were not reported consistently in the source literature. These variables were, therefore, not included because doing so would substantially reduce the usable dataset size.

Thermal conductivity was used only in the preliminary correlation analysis for records with paired thermal- and electrical-conductivity data. It was not included as an input descriptor in either electrical-conductivity prediction model. The final modelling dataset therefore contained 258 complete records characterized by five input variables and was used to examine associations between commonly reported material and processing descriptors and electrical conductivity in graphene–polymer composites.

2.2. Data preprocessing

Electrical conductivity values span more than seventeen orders of magnitude across the compiled dataset. To reduce the influence of extreme values and obtain a more balanced prediction target, conductivity was transformed as

$$y = \log_{10}(\sigma), \tag{1}$$

where σ is expressed in S/m. This logarithmic transformation is appropriate for conductivity data governed by percolation-like behavior, where small changes in graphene-network connectivity can lead to large changes in conductivity.

The dataset contains both categorical and numerical descriptors. Polymer matrix, filler type, processing route, and system classification were treated as categorical variables, whereas graphene loading was treated as a numerical variable. Graphene loading was standardized before model training according to

$$w_{\mathrm{std}} = \frac{w_{\mathrm{GNP}} - \mu_w}{s_w}, \tag{2}$$

where μ_w and s_w are the mean and standard deviation of graphene loading in the training data, respectively. The same transformation parameters were then applied to the test data to avoid information leakage.

2.3. Descriptive statistics

Table 1 summarizes the main characteristics of the compiled dataset. Graphene loading ranges from 0 to 30 wt%, indicating that the dataset includes both low-filled composites and highly filled systems. Electrical conductivity shows a much wider variation, ranging from 1×10^{-10} to 5.5×10^{7} S/m. This range, covering more than seventeen orders of magnitude, is consistent with the large conductivity changes commonly observed in graphene–polymer composites near the percolation transition.

The large mean and standard deviation of the raw conductivity values indicate that the distribution is highly skewed and strongly affected by high-conductivity samples. For this reason, the logarithmic conductivity $\log_{10}(\sigma)$ was used as the target variable in the machine-learning analysis. The dataset also contains diverse categorical descriptors, including 46 polymer matrices, 32 filler types, 69 processing routes, and 131 system classifications. This diversity reflects the heterogeneous nature of literature-reported graphene–polymer composites and supports the need for models that can account for both numerical and categorical variables.

Table 1. Overview and example records of the graphene–polymer composite dataset used in this study: (a) summary statistics of the complete compiled dataset; (b) ten example records showing the five input descriptors and the electrical-conductivity target.

Table 1(a) - Summary statistics

Variable	Type	Available N	Min	Max	Mean	Std / Unique
$wt\_GNP(\%)$	Continuous	475	0.000	30.000	3.197	4.651
σ (S/m)	Continuous	260	1.00×10^{-10}	5.50×10^{7}	2.09×10^{6}	8.20×10^{6}
Matrix	Categorical	486	–	–	–	46
Filler	Categorical	486	–	–	–	32
Process	Categorical	486	–	–	–	69
System	Categorical	486	–	–	–	131

Table 1(b) - Ten example records

ID	Polymer matrix	Filler type	Processing route	System classification	Graphene loading $wt\_GNP(\%)$	Electrical conductivity, σ(S/m)
1	Epoxy	GNP	Solution mix	Epoxy_GNP	0.1	1.00×10^{-6}
2	Epoxy	GNP	Solution mix	Epoxy_GNP	0.5	1.00×10^{-3}
3	Epoxy	GNP	Solution mix	Epoxy_GNP	1.0	1.00×10^{-1}
4	Epoxy	GO	Ultrasonic	Epoxy_GO	0.5	5.00×10^{-4}
5	Epoxy	GO	Ultrasonic	Epoxy_GO	1.0	2.00×10^{-2}
6	Epoxy	GNP	3-roll mill	Epoxy_GNP	2.0	1.00
7	Epoxy	GNP	3-roll mill	Epoxy_GNP	3.0	5.00
8	PP	GNP	Melt mix	PP_GNP	2.0	1.00×10^{-2}
9	PP	GNP	Melt mix	PP_GNP	5.0	5.00×10^{-1}
10	PVDF	GNP	Solution mix	PVDF_GNP	1.0	2.00×10^{-1}

To make the form of the modelling data more transparent, Table 1 also presents ten example records from the compiled dataset. Each record shows the five model inputs-polymer matrix, filler type, processing route, system classification, and graphene loading-together with electrical conductivity as the prediction target. These records are provided only to illustrate the organization of the dataset and do not constitute a separate subset used for model training or evaluation.

3. Methods

3.1. Physical background: electrical transport and percolation

Electrical conductivity in graphene–polymer composites is closely related to the formation of conductive pathways within the polymer matrix. At low graphene concentrations, the filler particles are usually separated from each other, and charge transport is limited by polymer barriers, interparticle spacing, and local tunnelling or hopping processes. A commonly used expression for tunnelling-controlled transport is

$$\sigma \propto \exp\left(-\frac{d}{\xi}\right), \tag{3}$$

where d is the average separation distance between neighboring graphene sheets and ξ is the tunnelling decay length.

When the graphene content approaches and exceeds the percolation threshold ϕ_c, connected graphene-rich pathways begin to form. In this regime, the conductivity is often described by the classical percolation scaling law,

$$\sigma \propto (\phi - \phi_c)^t, \tag{4}$$

where ϕ is the filler volume fraction and t is the transport exponent. These two limiting regimes help explain why electrical conductivity in graphene–polymer composites can change by many orders of magnitude over a relatively narrow range of filler loading.

The percolation process is affected not only by graphene content but also by microstructural factors such as lateral size, aspect ratio, reduction degree, dispersion state, agglomeration, orientation, and interflake contact. However, these descriptors are not reported consistently across the previous studies used to construct the present dataset. To preserve a sufficiently large dataset, the analysis therefore relies on variables that are available for most records: polymer matrix, filler type, processing route, system classification, and graphene loading. These descriptors do not measure the microstructure directly, but they can partly reflect differences in material composition and fabrication conditions that influence conductive-network formation.

3.2. Feature representation and statistical characterization

The model inputs consist of four categorical descriptors and one numerical descriptor. Polymer matrix, filler type, processing route, and system classification were treated as categorical predictors, while graphene loading was treated as a numerical predictor. In the tree-based models, categorical descriptors were retained as categorical variables rather than converted into arbitrary continuous numerical values.

Graphene loading was standardized using Eq. (2) before model training. The logarithmic conductivity defined in Eq. (1) was used as the prediction target.

On describing the shape of the numerical distributions, skewness and kurtosis were also calculated:

$$\text{Skewness} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{x_i - \mu_x}{s_x}\right)^3, \tag{5}$$

$$\text{Kurtosis} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{x_i - \mu_x}{s_x}\right)^4. \tag{6}$$

Skewness and kurtosis, defined in Eqs. (5) and (6), respectively, describe the asymmetry and degree of tail heaviness of the distribution. These statistics were used for dataset characterization, not as additional model inputs. Their inclusion helps clarify why conductivity was analyzed on a logarithmic scale and why nonlinear models are needed for this heterogeneous dataset.

Several physical descriptors that may affect percolation, including graphene aspect ratio, lateral size, dispersion quality, agglomeration state, orientation, and reduction degree, were not reported consistently in the source literature. These variables could not be included without substantially reducing the dataset size, and this limitation was considered in the interpretation of the model results.

3.3. Machine learning models

Two tree-based ensemble models, Random Forest (RF) and Gradient Boosting Regression (GBR), were used to predict the logarithmic electrical conductivity. These models were selected because the dataset contains both categorical and numerical descriptors and because the relationship between graphene loading, material descriptors, processing route, and conductivity is expected to be nonlinear. Tree-based models are also suitable for percolation-related data, where conductivity can change abruptly near the transition from isolated fillers to connected conductive pathways.

3.3.1. Random Forest

RF is an ensemble-learning method that combines many decision trees trained on bootstrap samples of the training data. In this study, the RF model was implemented using 400 decision trees**.** For each tree, the split at a given node was selected by reducing the mean squared error impurity. The impurity reduction can be written as

$$\Delta I = I_{\text{parent}} - \left(\frac{n_L}{n} I_L + \frac{n_R}{n} I_R \right) \tag{7}$$

where I_{parent} is the impurity of the parent node, I_L and I_R are the impurities of the left and right child nodes, and n, n_L, and n_R are the numbers of samples in the parent, left child, and right child nodes, respectively.

The prediction of the RF model is obtained by averaging the predictions of all trees:

$$\hat{y} = \frac{1}{N_{\text{tree}}} \sum_{i=1}^{N_{\text{tree}}} T_i(x). \tag{8}$$

where $T_i(x)$ is the prediction of the i-th tree for input x and N_{tree} is the total number of trees in the forest. Bootstrap sampling and ensemble averaging reduce the dependence on any single tree and help improve robustness when working with heterogeneous literature-derived data.

3.3.2. Gradient Boosting Regression

GBR is an ensemble-learning method that builds an additive model by fitting a sequence of regression trees. Unlike Random Forest, which trains trees independently, GBR adds trees sequentially so that each new tree reduces the prediction error remaining from the previous iteration. This makes GBR suitable for modelling nonlinear relationships between material descriptors and electrical conductivity.

At the m-th boosting iteration, the prediction is updated as

$$\hat{y}_m(x) = \hat{y}_{m-1}(x) + \eta h_m(x), \tag{9}$$

where $\hat{y}_m(x)$ is the prediction after the m-th iteration, $\hat{y}_{m-1}(x)$ is the prediction from the previous iteration, $h_m(x)$ is the regression tree fitted to the residual error at iteration m, and η is the learning rate.

In this study, the GBR model was implemented using 400 boosting iterations and a learning rate of 0.05. The base learners were regression trees with a minimum leaf size of 5 and a maximum of 40 splits per tree. These settings were used to control the complexity of individual trees while allowing the ensemble to capture nonlinear variations in $\log_{10}(\sigma)$ across different graphene loadings, polymer matrices, filler types, and processing routes.

3.3.3. Model training, validation, and evaluation

The dataset was randomly divided into training and testing subsets using an 80/20 hold-out split. A fixed random seed of 123 was used to ensure reproducibility of the data partition. The RF and GBR models were trained on the training subset and evaluated on the independent test subset. Five-fold cross-validation was additionally performed as a supplementary analysis to examine the stability of model performance across different data partitions.

Model performance was evaluated using the coefficient of determination (R^2), root mean squared error (RMSE), and mean absolute error (MAE):

$$R^2 = 1 - \frac{\sum_{i=1}^{N}\left(y_i - \hat{y}_i\right)^2}{\sum_{i=1}^{N}\left(y_i - \bar{y}\right)^2} \tag{10}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(y_i - \hat{y}_i\right)^2} \tag{11}$$

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}\left|y_i - \hat{y}_i\right| \tag{12}$$

Here, y_i, $\hat{y}_i$, and $\bar{y}$ denote the measured, predicted, and mean measured values of the target variable, respectively, and N is the number of samples. Since the prediction target is $\log_{10}(\sigma)$, RMSE and MAE represent errors on the logarithmic conductivity scale.

The computational workflow was implemented using conventional supervised machine-learning procedures; no prompt-based or large-language-model procedure was involved in model training, prediction, evaluation, or feature-importance analysis.

3.4. Feature importance and descriptor grouping

For the tree-based models, feature importance was calculated from the impurity reduction associated with each descriptor across the decision trees:

$$FI_j = \frac{\sum_{s:v(s)=j}\Delta I_s}{\sum_{k}\sum_{s:v(s)=k}\Delta I_s} \tag{13}$$

where ΔI_s is the impurity reduction at split s, and $v(s)$ is the descriptor used at that split.

To make the interpretation more consistent with composite-material concepts, individual feature importances were grouped into five descriptor groups: polymer matrix, filler type, processing route, system classification, and graphene loading.

The grouped importance of family g was then obtained as

$$FI_g = \sum_{j\in g} FI_j \tag{14}$$

The grouped analysis was used to examine how commonly reported descriptors are associated with conductivity variation. The grouped importance values were normalized relative to the total feature importance and are therefore reported as percentages in Fig. 6. The resulting importance values should be interpreted as model-based associations, not as direct measurements of physical mechanisms, because important microstructural descriptors such as aspect ratio, dispersion quality, reduction degree, orientation, and agglomeration state were not consistently available in the source literature.

4. Results and discussion

4.1. Distribution and percolation signature

The distribution of electrical conductivity, expressed as $\log_{10}(\sigma)$, is shown in Fig. 2. The data cover a wide range, from highly insulating to highly conductive systems. The histogram and KDE curve show a broad, non-normal distribution with two apparent conductivity regions. Most samples are located in the low-to-intermediate conductivity range, whereas a smaller group appears at much higher conductivity values.

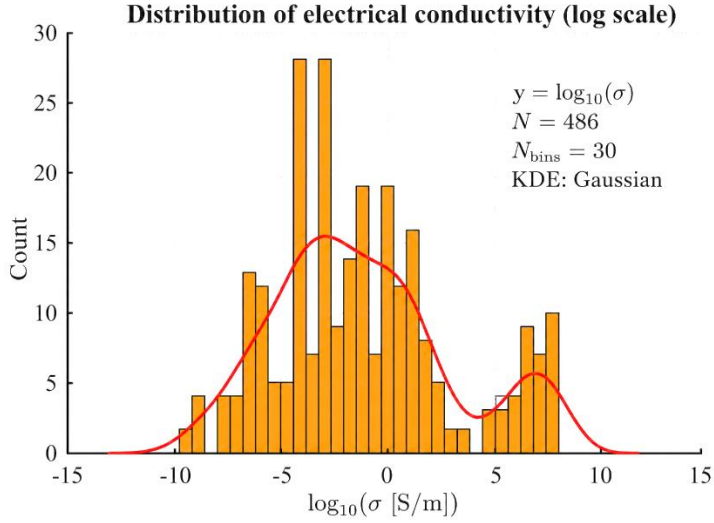

Figure 2. Distribution of $\log_{10}(\sigma)$ for the compiled graphene–polymer composite dataset. The histogram and KDE curve indicate a broad, non-normal distribution with two apparent conductivity regions.

This bimodal-like behavior is consistent with the coexistence of sub-percolated and percolated composite systems in the compiled dataset. In the low-conductivity region, graphene flakes are likely not sufficiently connected to form long-range conductive pathways, so charge transport may be limited by polymer barriers, interflake spacing, and local tunnelling or hopping processes. In contrast, the high-conductivity region is associated with samples in which graphene-rich pathways have become sufficiently connected to support long-range charge transport. This interpretation follows the classical picture of electrical percolation, where conductivity increases rapidly once the conductive filler network approaches a system-spanning state (Sahimi, 1996; Stauffer & Aharony, 1992), and is consistent with previous studies on graphene-based polymer composites (He & Tjong, 2013; Zare et al., 2024).

Figure 3 presents the Pearson correlation matrix among graphene loading, thermal conductivity, and $\log_{10}(\sigma)$. The strongest correlation is observed between thermal

conductivity and electrical conductivity $(r = 0,74)$, suggesting that both properties are partly influenced by the formation of graphene-rich transport pathways. By contrast, graphene loading shows almost no linear correlation with $\log_{10}(\sigma)$ $(r = -0.01)$. The weak negative correlation between graphene loading and thermal conductivity $(r = -0.24)$ also suggests that loading alone cannot explain the transport behavior across the compiled literature dataset.

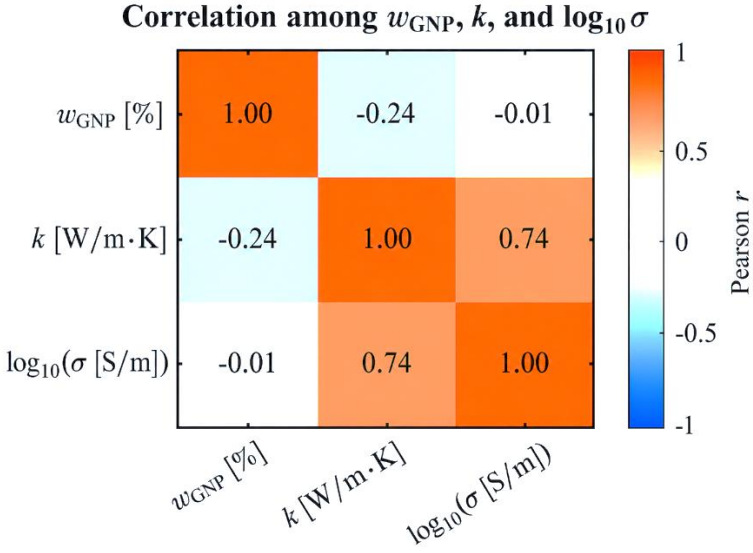

Figure 3. Pearson correlation matrix among graphene loading w_{GNP}, thermal conductivity k, and electrical conductivity expressed as $\log_{10}(\sigma)$. The coefficients represent linear pairwise correlations and should be interpreted with caution for nonlinear percolation-driven behavior.

Overall, Figs. 2 and 3 indicate that conductivity variation in graphene–polymer composites cannot be adequately described by a simple pairwise linear relationship. The data instead reflect combined effects of filler loading, matrix characteristics, filler properties, and processing-related factors. This result supports the use of multivariable nonlinear models, such as RF and GBR, for analysing conductivity trends across heterogeneous composite systems (Milad et al., 2022; Raza et al., 2025).

4.2. Dependence on graphene loading

Figure 4 shows the relationship between graphene loading and electrical conductivity on a log–log scale. The data are widely scattered, and the fitted power-law trend, $\sigma \propto w_{GNP}^{0.94}$, gives a very low coefficient of determination $(R^2 = 0.01)$. This result indicates that graphene loading alone cannot explain the large conductivity variation across the compiled dataset.

Although the global correlation is weak, the data suggest a percolation-like change in the low-loading region, approximately around 0.5–1 wt% GNP. This range is broadly consistent with reported percolation thresholds for graphene–polymer composites (He & Tjong, 2013; Zare et al., 2024). Below this region, graphene flakes are likely isolated or only locally connected, so charge transport is limited by polymer barriers, interflake spacing, and tunnelling or hopping processes (Sahimi, 1996; Stauffer & Aharony, 1992). At higher loadings, more connected graphene-rich pathways can form, leading to higher conductivity.

These results show that the relationship between graphene loading and electrical conductivity is nonlinear and exhibits substantial scatter across the compiled dataset. Figure 4 alone does not identify which material descriptors account for this scatter. This observation motivates the multivariable analysis presented in the following sections, in which polymer matrix, filler type, processing route, system classification, and graphene loading are considered jointly. This supports the use of multivariable nonlinear models, such as RF and GBR, for analysing conductivity trends in heterogeneous graphene–polymer composite datasets (Milad et al., 2022).

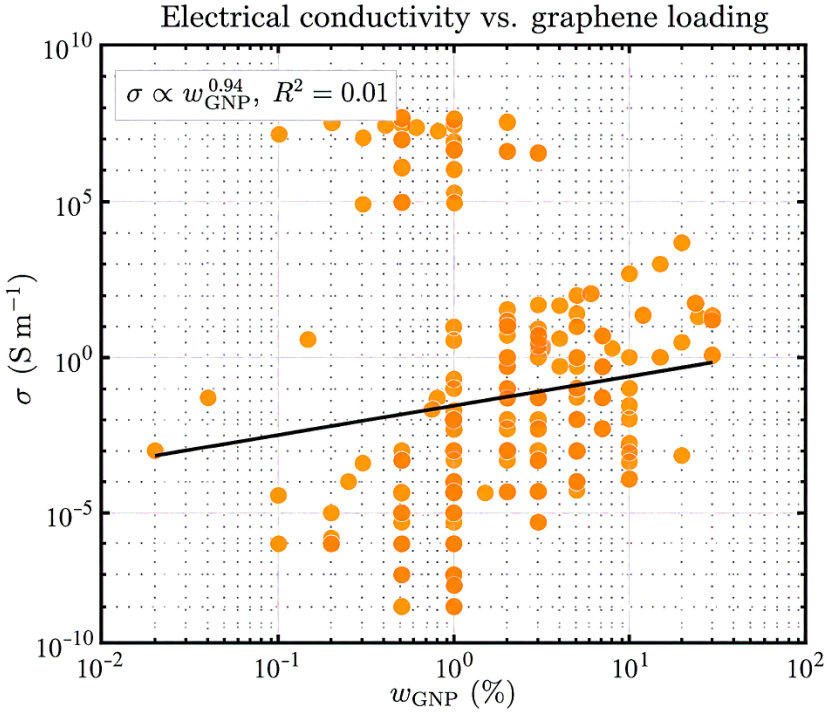

Figure 4. Dependence of electrical conductivity on graphene loading on a log–log scale. The weak global power-law fit $(R^2 = 0.01)$ indicates that graphene loading alone is insufficient to explain conductivity variation, although a percolation-like change is suggested in the low-loading region.

4.3. Model performance

Figure 5 compares the predicted and measured values of $\log_{10}(\sigma)$ for RF and GBR models. Both models reproduce the overall conductivity trend, but the predictions show different levels of scatter around the ideal $y = x$ line. RF achieves an R^2 of 0.84, with an RMSE of 1.77 and an MAE of 1.45. GBR gives better performance on the fixed test split, with an R^2 of 0.91, an RMSE of 1.36, and an MAE of 0.93 (Table 2).

Table 2. Predictive performance of Random Forest and Gradient Boosting Regression models for $\log_{10}(\sigma)$ on the fixed test split, where σ is expressed in S/m.

Model	R^2	RMSE	MAE
Random Forest	0.84	1.77	1.45
Gradient Boosting	0.91	1.36	0.93

The parity plots show that GBR predictions are closer to the ideal line, especially in the intermediate- and high-conductivity ranges. This suggests that GBR captures the nonlinear conductivity variation more effectively than RF for this dataset. However, deviations remain for some samples, particularly near the percolation transition region. In this region, small differences in dispersion quality, interflake contact, and conductive-network formation can produce large changes in conductivity.

Overall, the selected descriptors, including polymer matrix, filler type, processing route, system classification, and graphene loading, contain useful information for predicting electrical conductivity. At the same time, the remaining errors reflect the limitations of literature-derived data, where important microstructural variables such as graphene aspect ratio, dispersion quality, reduction degree, orientation, and agglomeration state are not consistently reported.

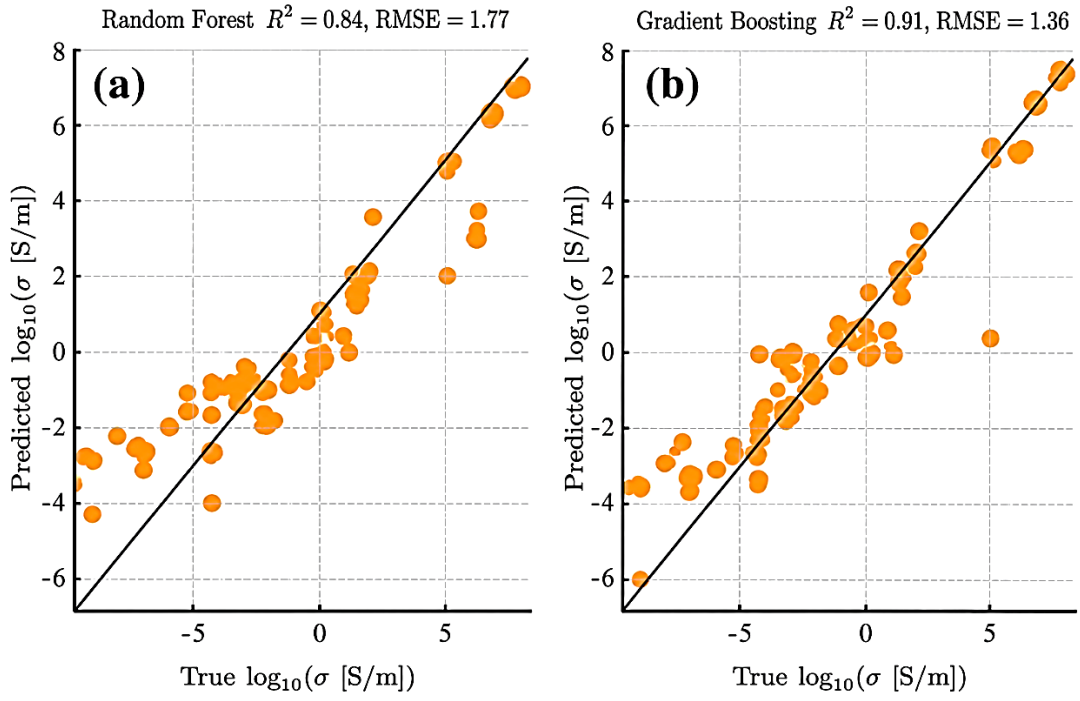

Figure 5. Parity plots for predicting $\log_{10}(\sigma)$ using (a) Random Forest and (b) Gradient Boosting on the fixed test split. Each point compares predicted and measured values, and the dashed line indicates the ideal $y = x$ relationship. Gradient Boosting shows higher accuracy $(R^2 = 0.91)$ and lower error than Random Forest $(R^2 = 0.84)$.

4.4. Feature importance and physical interpretation

Grouped feature importance analysis was used to examine the relative contribution of the main descriptor families to conductivity prediction (Fig. 6). Graphene loading shows the highest grouped importance, accounting for 34.1% of the total normalized importance, followed closely by system classification at 32.6%. Processing route contributes 20.8%, whereas polymer matrix and filler type contribute 9.1% and 3.2%, respectively. These percentages represent the relative shares of the total model-based feature importance assigned to each descriptor group; they do not represent the percentage of electrical conductivity physically explained by each variable and should not be interpreted as causal contributions.

The relatively high importance of graphene loading is physically reasonable because filler concentration controls the proximity of a composite to the formation of a connected conductive network. However, its importance of 34.1% also indicates that graphene loading alone does not dominate the model prediction. The comparable contribution of system classification (32.6%) suggests that broader differences among composite systems contain substantial predictive information. Processing route contributes a further 20.8%, consistent with the physical role of fabrication conditions in controlling graphene dispersion, interflake contact, platelet orientation, and conductive-network formation (Kim et al., 2010; Kuilla et al., 2010; Ladani et al., 2015; Tarhini & Tehrani-Bagha, 2023).

Polymer matrix and filler type show lower grouped importances of 9.1% and 3.2%, respectively. These lower values should not be interpreted as evidence that matrix and filler characteristics are physically unimportant. Matrix-dependent properties such as polarity, viscosity, chain mobility, and interfacial compatibility can influence the development of conductive pathways, while filler characteristics may reflect differences in graphene morphology, reduction state, layer number, and surface chemistry (Sun et al., 2022). Within the present literature-derived dataset, however, part of this predictive information may overlap with broader descriptors such as system classification and processing route. Moreover, important microstructural variables such as graphene aspect ratio, dispersion quality, reduction degree, orientation, and agglomeration state were not consistently available in the source literature (Zare et al., 2024).

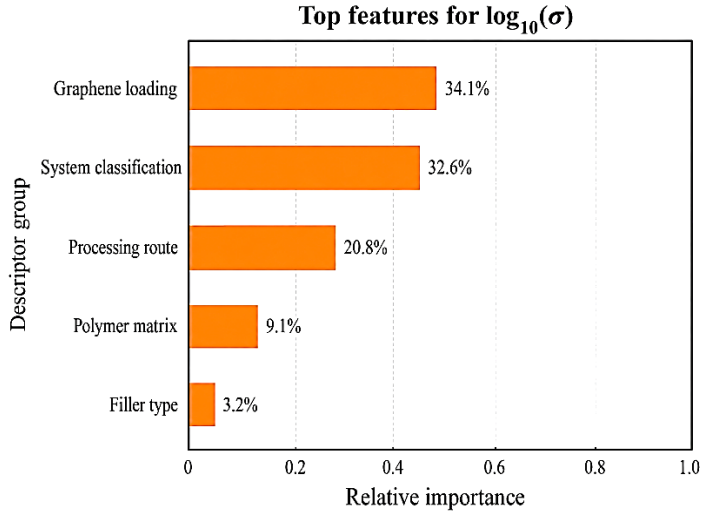

Figure 6. Normalized grouped feature importance for predicting $\log_{10}(\sigma)$. Descriptor groups are shown in descending order of importance: graphene loading (34.1%), system classification (32.6%), processing route (20.8%), polymer matrix (9.1%), and filler type (3.2%). Percentages represent each descriptor group's relative share of the total model-based feature importance.

Overall, the grouped importance analysis indicates that conductivity prediction in the present dataset is distributed across several descriptor groups rather than being controlled by graphene loading alone. This is consistent with the physical picture in which electrical transport depends not only on filler concentration but also on the spatial organization and connectivity of the graphene network (Sahimi, 1996; Stauffer & Aharony, 1992; Raza et al., 2025). Nevertheless, the feature-importance values should be interpreted as model-based associations rather than direct physical measurements or causal effects. Their magnitude

depends on the available descriptors, their statistical structure, and the composition of the compiled dataset.

From a practical viewpoint, the results suggest that conductivity optimization should not rely only on increasing graphene loading. Processing route, matrix selection, and filler quality should be considered together because they affect dispersion, interflake contact, and conductive-network formation. The proposed modelling approach can therefore support preliminary screening of material and processing combinations before more detailed experimental optimization.

5. Conclusions

This study analyzed a literature-derived dataset of 486 graphene–polymer composite records using RF and GBR models. Electrical conductivity was modeled as $\log_{10}(\sigma)$ because the reported values span a very wide range. The conductivity distribution showed distinct low- and high-conductivity regimes, consistent with the coexistence of sub-percolated and percolated composite systems.

Both models reproduced the main conductivity trend, with GBR giving better performance on the fixed test split. The results indicate that polymer matrix, filler type, processing route, system classification, and graphene loading contain useful information for predicting electrical conductivity. The grouped feature-importance analysis shows that graphene loading and system classification provide the largest relative contributions to the model predictions, followed by processing route, while polymer matrix and filler type show lower grouped importance. These results indicate that conductivity prediction is distributed across several descriptor groups rather than being controlled by graphene loading alone.

The analysis also shows that graphene loading alone is insufficient to explain conductivity variation across heterogeneous literature data. Similar filler contents can lead to different conductivities because of differences in dispersion, filler quality, interflake contact, and matrix–filler interactions. Since microstructural descriptors such as aspect ratio, dispersion quality, reduction degree, and agglomeration state were not consistently available in the source literature, the model outputs should be interpreted as trends within the compiled dataset rather than universal predictions for all graphene–polymer composites.

From a practical viewpoint, the results suggest that conductivity optimization should consider processing route, matrix selection, and filler quality together with graphene loading. The modelling approach can support preliminary screening of material and processing combinations before detailed experimental optimization. Future studies would benefit from more consistent reporting of graphene morphology, dispersion state, processing conditions, and measurement protocols to improve both predictive accuracy and physical interpretation.

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