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A Hybrid Multi-Physics Ensemble Deep Learning Framework for Simultaneous Prediction of Thermal and Electrical Conductivity in Functional Polymer-Based Nanocomposites

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Abstract

Polymer-based nanocomposites have become promising materials for applications in energy storage, flexible electronics, biomedical devices, aerospace components, and advanced engineering because of their tunable thermal and electrical properties. Reliable prediction of these properties is essential for accelerating material design; however, existing analytical models and conventional machine learning techniques often fail to represent the complex interactions among filler characteristics, polymer matrices, processing conditions, and interfacial transport phenomena. This work presents HMEP-Net, a Hybrid Multi-Physics Ensemble Prediction Network developed to improve the simultaneous prediction of thermal and electrical conductivity in functional polymer nanocomposites. The proposed framework integrates physics-guided conductivity descriptors with deep feature extraction through an auto encoder, followed by CNN-BiLSTM learning, an attention-based feature fusion mechanism, and an adaptive ensemble meta-learning strategy. By combining physical knowledge with data-driven learning, the framework captures both transport mechanisms and nonlinear material relationships more effectively than existing approaches. The predictive capability of HMEP-Net was evaluated against Linear Regression, Support Vector Regression, Random Forest, XGBoost, Deep Neural Networks, CNN-LSTM, and Attention-CNN-BiLSTM models. The proposed method achieved the highest prediction accuracy, yielding an MAE of 0.041, RMSE of 0.061, and R^2 of 0.985 for thermal conductivity, together with an MAE of 0.047, RMSE of 0.069, and R^2 of 0.983 for electrical conductivity. Robustness analysis further demonstrated stable performance under 20% noises, with R^2 values remaining above 0.96 for both prediction tasks. These results indicate that HMEP-Net provides a reliable and computationally efficient framework for conductivity prediction and supports the accelerated design and optimization of next-generation polymer-based nanocomposite materials.

Keywords: Polymer nanocomposites, thermal conductivity prediction, electrical conductivity prediction, deep learning, attention mechanism, ensemble learning and materials informatics

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INTRODUCTION

Polymer-based nanocomposites are one of the most important families of innovative materials due to their lightweight structure, high mechanical performance, thermal stability, and tunable electrical properties [1]. These materials are used in energy storage systems [2], flexible electronics, electromagnetic shielding, biomedical devices, aircraft constructions, and automotive components [3]. Conductive Nano-fillers like carbon nanotubes, graphene, nano-clays, metallic nanoparticles, and hybrid nanostructures improve thermal and electrical conductivity in polymer matrices while maintaining desirable material properties [4–5].

Complex relationships between filler concentration, particle shape, aspect ratio, surface functionalization, processing factors, and environmental conditions affect polymer nanocomposites [6]. Phonon propagation through matrix-filler interfaces affects thermal transport, while conductive route creation and percolation affect electrical conductivity [7]. Predicting conductivity behaviour accurately is difficult because tiny changes in material composition or processing conditions can drastically influence transport properties [8–9].

Maxwell-Garnett theory, Bruggeman models, and percolation-based analytical formulations provide physical insights into conductivity mechanisms [10–11]. Filler dispersion, isotropy, and interfacial interactions are usually simplified in these methods. They lose prediction accuracy in complicated nanocomposite systems with many fillers, hybrid reinforcements, or nonlinear processing effects [12].

Recent improvements in machine learning enable data-driven material property prediction. Support Vector Regression, Random Forests, Artificial Neural Networks, and Gradient Boosting simulate nonlinear material behaviour well [13–14]. Additionally, deep learning architectures like CNNs, LSTMs, and attention-based models may extract complex feature correlations [15]. Despite these advances, many conductivity transfer models use statistical correlations and ignore the physical mechanisms [16]. This constraint may reduce interpretability, generalisation, and physical consistency.

A Hybrid Multi-Physics Ensemble Prediction Network (HMEP-Net) that mixes physical conductivity theories with sophisticated deep learning and ensemble learning methodologies is proposed to address these issues. The proposed system captures physical and statistical correlations in polymer nanocomposite datasets via physics-guided conductivity encoding, deep feature compression, CNN-BiLSTM hybrid learning, attention-based feature fusion, and adaptive ensemble optimisation. The suggested model predicts thermal and electrical conductivity while keeping physically important transport features, unlike current methods.

This research makes three key contributions. First, thermal and electrical transport concepts are directly integrated into learning via a physics-guided feature representation technique. Second, hybrid deep learning architectures capture local interactions, long-range interdependence, and feature importance. Third, an ensemble meta-learning framework reduces uncertainty and improves prediction resilience. HMEP-Net strives to deliver an accurate, interpretable, and computationally economical solution for next-generation conductivity prediction and material informatics.

Rest of the paper is organized as follows: Section 2 discusses related works, Section 3 details proposed methodology, Section 4 analyses the results, and Section 5 concludes.

RELATED WORKS

Lakshmaiya et al. [17] propose a physics-informed data-driven approach for building a high-fidelity surrogate model for accurate prediction of in-plane along with through-plane silver nanoparticles. A detailed secondary dataset from published experimental studies including filler quality, hybrid ratios,

processing parameters, alignment approaches and anisotropic conductivity responses. Python was used to train a Deep Neural Network surrogate, after extensive preprocessing steps which include missing-value imputation, min–max normalisation and composite-specific engineered descriptors with stratified data splits, The Orientation Anisotropy Index, Interfacial Surface Density and Synergistic Hybrid Factor were constructed to signify directional heat-flow pathways, matrix–filler thermal coupling and cooperative multi-filler effects respectively Architectural depth along with generalisation were optimised using Bayesian Optimisation with an acquisition function of Gaussian Improvement. This approach has improved the predictive architecture by optimising the hyper parameter space exploration. The optimised DNN has R^2 = 0.99995, RMSE and MAE reduced to 0.00131 and 0.000998, beating baseline models (e.g. Gradient Boosting Decision Tree, Multi-Layer Perceptron and FFANN) (≈12–18% accuracy gain). Bayesian- physics-consistent prediction engine to accelerate composite design and drive manufacturing operations in next-generation thermal interface resources.

Sharma, H., et al. [18] used machine learning to estimate the hardness and tensile strength of PP/CNT and LDPE/CNT composite materials. Microwave-assisted manufacturing was used to make the composites, which were tested at 100 °C, below the melting temperatures of PP and LDPE. A universal testing machine and Rockwell hardness tester were used for tensile and hardness tests. ML techniques like XGBoost, KNN, and RF predicted these features. RF was the most accurate and consistent, especially for PP/CNT composites. RMSE, MAE, and R2 showed that the RF model outperformed other techniques. The hardness and tensile strength of PP/CNT composites showed minimum fluctuations of 0.5 and 2, respectively, indicating remarkable predictive accuracy. In contrast, LDPE/CNT composites had higher variances of ±1 and ±3 due to a lower correlation between anticipated and experimental values. This study shows that ML, specifically the RF algorithm, can accurately predict composite material properties.

Madani and Abbasi [19] create solid data-driven models using 1447 experimental points. The dataset includes 25–90 °C temperatures, 0.1–15 wt% polymer concentrations, 0.1–1 wt% nanoparticle concentrations, and 9.75-1021.38 s−1 shear rates. Temperature, polymer and xanthan gum) and nanoparticles are inputs. Viscosity was 1.30–2160 cP. The dataset comprises polymer systems with and without nanoparticles, allowing models to capture viscosity differences before and after nanoparticle integration. Nanoparticle addition increases viscosity through particle–polymer interactions, but the extent depends on shear rate, polymer content, and nanoparticle type. Decision Tree, Random Forest, AdaBoost, K-Nearest Neighbours, CNN, and Ensemble Learning were used. Shear rate affected viscosity most, while nanoparticle type had the least impact, according to SHAP study. Leverage identified 18 outliers in data quality, however all points were kept for modelling. 5-fold cross-validation trained and validated models. AdaBoost (depth 9) fared best with R2 values %. CNN performed worst. Ensemble Learning increased accuracy (R2 = 0.999191, MSE = 74.49). Cross-plots and error distribution analysis verified the top models' dependability and robustness. These results demonstration ensemble learning approaches, particularly AdaBoost then Random Forest may accurately and scalable estimate EOR system viscosity. The models efficiently screen and assist viscosity estimates and nano–polymer composite optimisation in laboratory circumstances relevant to enhanced oil recovery.

Zhang, F., et al. [20] layered polyamide epichlorohydrin graphene Nano sheets (pGNPs) within silver nanoparticles deposited CNFs finished electrostatic self-assembly via vacuum filtration to create composites with high thermal conductivity (TC) and electromagnetic interference shielding efficiency (EMI SE). After hot-pressing, CNFs-based composites with “mimosa”-like ordered layered constructions have densely interconnected pGNPs with a TC of 150.6 W/(m K) and an EMI SE of 75 dB. By combining CNFs-based composites with excellent Joule heating curtains and grabbers with 82° bending angles under 3 V are produced. A composite made of CNFs with high conductivity (9.8 103 S m1) is utilised as an electrode in turboelectric Nano generators for Morse code transmission.

The as-prepared CNFs-based composites can extend actuator and sensor life, enabling multi-functional wearable terminals then biomimetic actuators.

Du, H., et al. [21] offer a unified numerical outline that uses the MC approach to statistically forecast inter-CNT distances and the EMA method to efficiently estimate the composite's macroscopic conductive characteristics. The poor matrix-CNT bonding and electron tunnelling between nearby CNTs are described by an interface model. The integrated technique efficiently captures the percolation threshold and macroscopic conductive behaviour while physically modelling tunnelling conductivity. The model's accuracy and the importance of CNT are confirmed by experimental data.

Hegazy, M. A., et al. [22] report that these metal oxides (MOs) improve active sides and surface area for humidity detection, but nothing is known about their impacts on critical polymer composition and humidity sensitivity. A theoretical study examined how different MOs affect Polyvinyl Alcohol (PVA) matrix sensitivity, stability, and electrical properties. MOs and PVA matrix interact to build new active chemical groups, enhancing PVA sensitivity and reactivity. PVA's higher surface energy causes reactivity, and ZnO Nano filler is the best modification. By incorporating new ingredients like graphene (G), PVA-ZnO-based sensors can immediately improve surface reactivity and humidity finding sensitivity. The PVA-ZnO-G hybrid nanocomposites surface, intermolecular, reactivity, hardness, softness, sensitivity, and selectivity were examined for humidity sensing. When compared to the PVA-ZnO-G-5H2O combination, the latter has better electrical properties. It has a higher dipole moment of 21.0848 Debye, a lower band gap of 0.503 eV, and a better adsorption energy of -0.7592 eV. The rise in equilibrium constant (log K = 12.8380) suggests that PVA-ZnO-G is thermodynamically feasible and has improved stability and sensitivity. The hybridisation of ZnO and the introduction of G into the matrix improved mechanical, thermal, and electrical properties and boosted H2O interaction.

PROPOSED HMEP-NET FRAMEWORK

Thermal and electrical conductivity in functional polymer-based nanocomposites are difficult to predict due to highly nonlinear interactions between matrix materials, conductive fillers, interfacial regions, processing conditions, and microstructural evolution. Maxwell-Garnett, Bruggeman, and percolation-based models provide useful physical insights but often fail to capture the complex interactions in heterogeneous nanocomposite systems, especially when multiple fillers, surface modifications, and processing-induced anisotropies are present. Conventional machine learning models may neglect essential heat and charge transport pathways since they only use statistical relationships. Proposed model architecture is shown in Figure 1.

Hybrid Multi-Physics Ensemble Prediction Network (HMEP-Net) addresses these issues. Physical conductivity theories, deep learning, and ensemble learning are used to map material attributes to conductivity responses. The model has seven interconnected stages, from multi-source feature representation to multi-objective conductivity prediction. The design continuously transforms raw nanocomposite descriptors into more useful latent representations while maintaining physical consistency during prediction.

The suggested framework's mapping function is

$$\hat{Y} = F(X; \Theta) \tag{1}$$

where $X = \{x_1, x_2, \ldots, x_n\}$ characterizes the input feature vector, Θ represents all trainable parameters of the framework, and $\hat{Y} = [\hat{k}, \hat{\sigma}]$ characterizes the predicted thermal conductivity and electrical conductivity simultaneously.

The complete model seeks to approximate the nonlinear transformation

$$F: \mathbb{R}^n \rightarrow \mathbb{R}^2 \tag{2}$$

where material composition, filler properties, and manufacturing conditions predict conductivity.

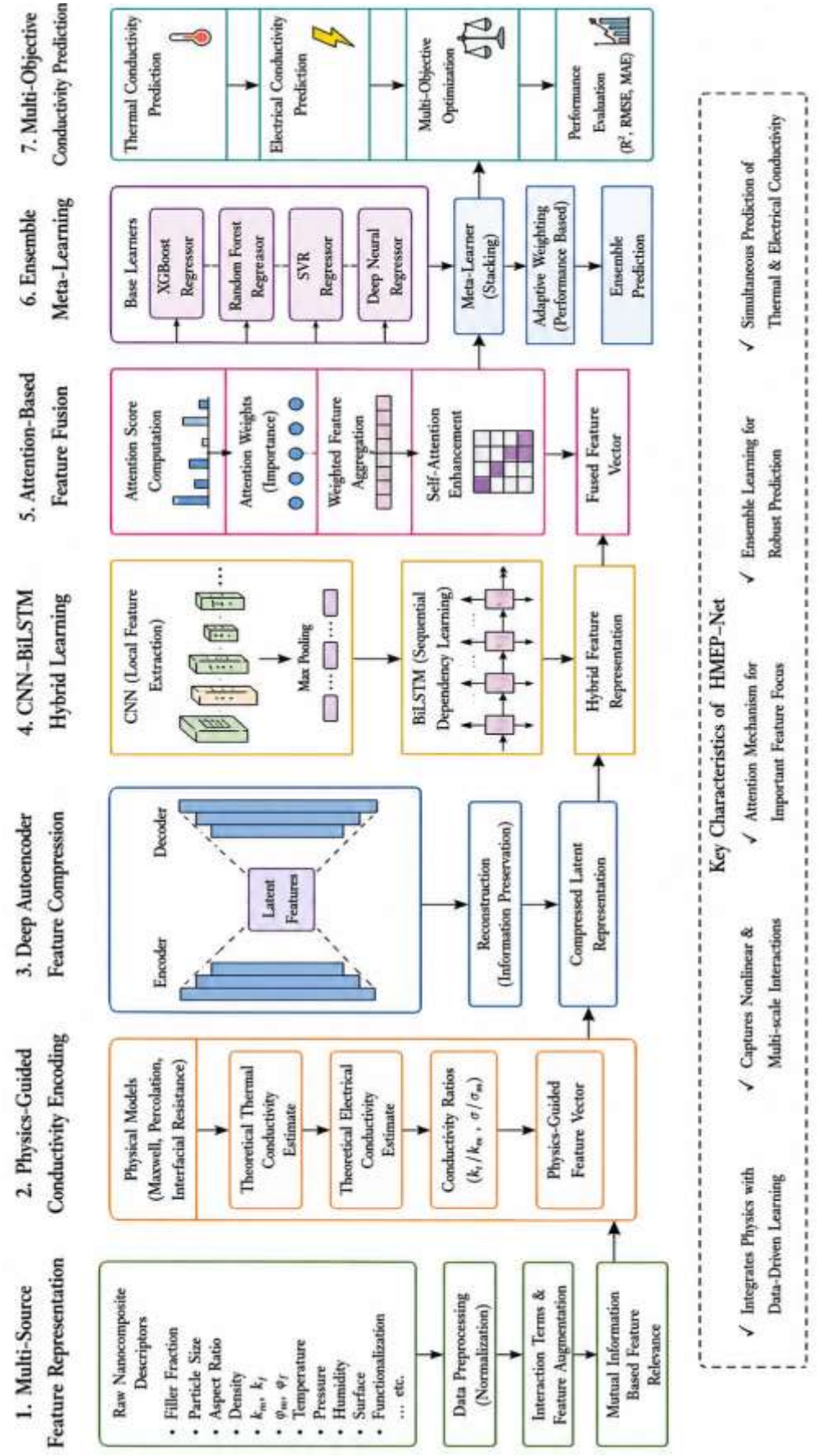

Figure 1. Architecture of the proposed model.

Multi-Source Nanocomposite Feature Representation

Machine learning systems' predictive power depends on their feature representation. Material characteristics affect polymer nanocomposites' conductivity from molecular interactions to macroscopic structural organization. Thus, the framework initially creates a feature space with compositional, structural, processing, and environmental descriptors.

Initial feature vector is

$$X = \{\phi, d_p, AR, \rho, k_m, k_f, \sigma_m, \sigma_f, T, P, RH, S_f\} \quad (3)$$

Where ϕ= filler volume fraction, d_p= nanoparticle diameter, AR= aspect ratio, ρ= density, k_m= matrix thermal conductivity, k_f= filler thermal conductivity, σ_m= matrix electrical conductivity, σ_f= filler electrical conductivity, T= operating temperature, P= processing pressure, RH= relative humidity, S_f= surface functionalization coefficient.

Direct usage would bias model learning because these variables have different scales and units. Normalisation uses z-score standardisation.

$$X_i' = \frac{X_i - \mu_i}{\sigma_i} \quad (4)$$

Where μ_i mean value of feature i, $\sigma_i$is the standard deviation. The normalized dataset becomes

$$X' = \{x_1', x_2', \ldots, x_n'\} \quad (5)$$

which ensures equal feature contribution during training. To enhance representation of inter-feature relationships, pairwise interaction terms are produced as $I_{ij} = x_i' x_j'$ for $i \neq j$ thereby allowing the framework to capture coupling effects between composition and morphology.

For example, $I_{\phi,AR} = \phi \times AR$ quantifies the combined influence of filler loading and particle geometry on conductive network formation.

$$X_A = [X', I] \quad (6)$$

where I denotes all interaction features. To quantify feature relevance, mutual information scores are computed.

$$MI(X_i, Y) = \sum p(x_i, y) \log \left(\frac{p(x_i, y)}{p(x_i)p(y)}\right) \quad (7)$$

Where Y represents conductivity targets. Because they anticipate target behaviour, features with more mutual information predict conductivity better.

The representation lays the groundwork for physics-guided conductivity encoding.

Physics-Guided Conductivity Encoding

Data-driven learning may produce predictions that defy physics. Conductivity theory is immediately included into feature representation to avoid contradictions. Thermal conductivity prediction begins with Maxwell theory's effective conductivity estimate.

$$k_{eff} = k_m \left(\frac{k_f + 2k_m + 2\phi(k_f - k_m)}{k_f + 2k_m - \phi(k_f - k_m)}\right) \quad (8)$$

Where k_{eff} characterizes the theoretical effective conductivity. The equation captures how filler loading influences thermal transport through matrix-filler interactions.

$$k_{mod} = \frac{k_{eff}}{1 + R_K k_{eff}} \quad (9)$$

Where R_K represents Kapitza thermal resistance. Heat transport barriers at matrix-filler interfaces

are better represented with this adjustment. Similarly, percolation theory models electrical conductivity.

$$\sigma_{eff} = \sigma_0(\phi - \phi_c)^t \quad (10)$$

for $\phi > \phi_c$ Where σ_0= conductivity coefficient, ϕ_c= percolation threshold, t= critical exponent. Below the threshold, $\sigma_{eff} = 0$ indicating the absence of a continuous conductive pathway. The physical conductivity descriptors are incorporated into the feature vector.

$$X_P = [X_A, k_{mod}, \sigma_{eff}] \quad (11)$$

Experimental features and physically derived conductivity indicators are incorporated in the richer representation. To describe transport efficiency, conductivity ratio is added.

$$CR = \frac{k_f}{k_m} \quad (12)$$

Similarly,

$$ER = \frac{\sigma_f}{\sigma_m} \quad (13)$$

The ratios show conductivity differences between fillers and matrix materials. Finally, physics-guided representation becomes

$$X_{PG} = [X_P, CR, ER] \quad (14)$$

Before deep learning, the network has physically meaningful conductivity.

Deep Auto encoder-Based Feature Compression

The prior stage's physics-guided feature representation greatly enhances input space description. Compositional descriptors, interaction terms, conductivity ratios, theoretical conductivity estimates, and ambient variables create a high-dimensional feature space with redundant, correlated, and noisy information. Such redundancy can adversely affect model convergence, increase computational complexity, and reduce generalization performance. Therefore, an efficient feature compression mechanism is required before deep predictive learning can be performed.

The proposed HMEP-Net employs deep auto encoder architecture to transform the high-dimensional physics-guided feature space into a compact latent representation while preserving the most informative dimensionality reduction techniques such as Principal Component Analysis (PCA), which assume linear relationships among variables, auto encoders can capture nonlinear dependencies frequently encountered in polymer nanocomposite systems.

Let the physics-guided feature vector be represented as

$$X_{PG} = [x_1, x_2, \dots, x_d] \quad (15)$$

Where d denotes the total number of input features after augmentation. The encoder transforms the original feature space into a lower-dimensional latent representation through successive nonlinear mappings. The first hidden layer is expressed as

$$h_1 = f(W_1 X_{PG} + b_1) \quad (16)$$

Where W_1 represents the weight matrix, b_1 represents the bias vector, and $f(\cdot)$ denotes the activation function. A Rectified Linear Unit (ReLU) activation is adopted owing to its computational efficiency and ability to mitigate gradient vanishing.

$$f(z) = \max(0, z) \quad (17)$$

The second hidden layer becomes

$$h_2 = f(W_2 h_1 + b_2) \tag{18}$$

Encoding continues until a compact latent representation is produced.

$$z = f(W_e h_{L-1} + b_e) \tag{19}$$

Where $z = [z_1, z_2, \dots, z_m]$ And $m < d$. Nanocomposite behaviour is condensed in the latent vector. The decoder reconstructs the feature space to preserve conductivity information.

$$\hat{h}_{L-1} = f(W_d z + b_d) \tag{20}$$

Subsequent decoding layers generate

$$\hat{X} = g(W_o \hat{h}_1 + b_o) \tag{21}$$

Where $\hat{X}$ represents the input vector rebuilt. The reconstruction goal minimises information loss between original and recreated representations.

$$L_{rec} = \frac{1}{N} \sum_{i=1}^{N} \| X_i - \hat{X}_i \|^2 \tag{22}$$

Where N signifies number of samples. To prevent over fitting and encourage sparse representations, an L_2 regularization term is incorporated.

$$L_{reg} = \lambda \sum_{j=1}^{P} w_j^2 \tag{23}$$

Where P characterizes the total sum of trainable parameters. The complete auto encoder objective converts

$$L_{AE} = L_{rec} + L_{reg} \tag{24}$$

The optimization process updates parameters rendering to

$$\theta^{t+1} = \theta^t - \eta \nabla_\theta L_{AE} \tag{25}$$

Where η represents the learning rate. The resulting latent representation

$$Z = [z_1, z_2, \dots, z_m] \tag{26}$$

comprises compressed structural, compositional, thermal, and electrical data. The compact feature space reduces noise and improves computational efficiency for deep learning.

Latent feature relevance is quantified via variance contribution analysis.

$$VC_j = \frac{Var(z_j)}{\sum_{i=1}^{m} Var(z_i)} \tag{27}$$

Where VC_j signifies the contribution of latent feature j. Features exhibiting larger variance charities contain greater discriminatory power for conductivity prediction. The final compressed illustration is uttered as

$$Z^* = \{z_1, z_2, \dots, z_m\} \tag{28}$$

which serves as the direct input to the hybrid learning module.

CNN–BiLSTM Hybrid Learning Module

Although the latent feature representation successfully removes redundancy, Complex interplay between structural, compositional, and processing variables control polymer nanocomposites' conductivity. A learning technique that extracts local nonlinear patterns and long-range interdependence is needed to capture these interactions. Thus, the proposed approach combines CNNs and BiLSTMs into a single learning architecture.

CNN detects localised feature interactions related to conductivity mechanisms such filler clustering, conductive path creation, and interfacial transfer. The latent vector is initially arranged into a one-dimensional feature sequence.

$$Z^* = [z_1, z_2, \dots, z_m] \tag{29}$$

A convolution operation is then applied.

$$F_j = f\left(W_j * Z^* + b_j\right) \tag{30}$$

Where $*$ signifies convolution. The resulting feature map captures local conductivity-related structures. For kernel size k, the convolution can be expressed as

$$F_j(t) = \sum_{i=0}^{k-1} W_i Z_{t+i} + b_j \tag{31}$$

Pooling created feature maps reduces dimensionality while keeping dominant conductivity.

$$P_j = \max(F_j) \tag{32}$$

where max-pooling selects strongest activation. After pooling, CNN output becomes

$$P = [P_1, P_2, \dots, P_r] \tag{33}$$

Where r denotes the number of filters.

CNNs can discover local interactions but not long-range relationships between distant features. Filler functionalization may affect conductivity only with certain volume fractions and processing temperatures. Such relationships demand progressive learning. Pooled features are sent to a LSTM network. The forward concealed state is calculated as

$$\overrightarrow{h_t} = LSTM(P_t, \overrightarrow{h_{t-1}}) \tag{34}$$

while backward hidden state becomes

$$\overleftarrow{h_t} = LSTM(P_t, \overleftarrow{h_{t+1}}) \tag{35}$$

The final BiLSTM illustration is obtained through concatenation.

$$h_t = [\overrightarrow{h_t}; \overleftarrow{h_t}] \tag{36}$$

Within each LSTM unit, the forget gate determines which material should be retained.

$$f_t = \sigma(W_f[h_{t-1}, x_t] + b_f) \tag{37}$$

The input gate determines statistics enters memory.

$$i_t = \sigma(W_i[h_{t-1}, x_t] + b_i) \tag{38}$$

The candidate memory state is intended as

$$\tilde{C}_t = \tanh(W_c[h_{t-1}, x_t] + b_c) \tag{39}$$

The memory cell is updated according to

$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t \tag{40}$$

Where $\odot$ characterizes element-wise multiplication. The output gate

$$o_t = \sigma(W_o[h_{t-1}, x_t] + b_o) \tag{41}$$

and the hidden state is obtained as

$$h_t = o_t \odot \tanh(C_t) \tag{42}$$

This architecture enables simultaneous preservation of local conductivity patterns and long-range

nonlinear dependencies. To further improve feature discrimination, a residual connection is introduced.

$$R_t = h_t + P_t \tag{43}$$

Residual learning stabilizes gradient propagation and ensures retention of physically meaningful conductivity information extracted by the convolutional stage. The final hybrid representation generated by the CNN–BiLSTM module becomes

$$H = [R_1, R_2, \dots, R_T] \tag{44}$$

Where T denotes the sequence length. This representation contains enriched information describing conductive network formation, filler dispersion characteristics, interface effects, thermal transport mechanisms, and charge transfer behavior. Consequently, the subsequent attention-based fusion mechanism can selectively emphasize the most influential conductivity predictors before ensemble learning and final conductivity estimation.

Attention-Based Feature Fusion Strategy

In the preceding section, the CNN–BiLSTM learning module created a hierarchical representation including local conductivity patterns, long-range dependencies, and nonlinear nanocomposite descriptor interactions. Not every extracted trait predicts thermal and electrical conductivity equally. In actual polymer nanocomposite systems, filler volume percentage, conductive network density, interfacial resistance, and aspect ratio are more important. Thus, giving all learnt features identical weight may reduce prediction performance and add noise to conductivity estimation.

The proposed HMEP-Net uses attention-based feature fusion to overcome this problem. The attention module dynamically weights collected features based on their conductivity prediction contribution. This method lets the framework prioritise conductivity-related representations and suppress irrelevant ones. Represent CNN–BiLSTM output as

$$H = [h_1, h_2, \dots, h_T] \tag{45}$$

Where $h_t \in \mathbb{R}^{d_h}$ signifies the hidden representation at position t, and d_h characterizes the hidden feature dimension. The first step computes an attention score for each hidden representation.

$$e_t = v^T \tanh\left(W_a h_t + b_a\right) \tag{46}$$

Where W_a is the attention weight matrix, b_a the bias vector, and v the trainable attention projection vector. The scalar value e_t quantifies feature representation h_t's conductivity prediction importance. These scores are not normalised, thus a softmax function converts them to probability distributions.

$$\alpha_t = \frac{\exp\left(e_t\right)}{\sum_{j=1}^{T} \exp\left(e_j\right)} \tag{47}$$

Where α_t characterizes the normalized attention coefficient. The normalization process ensures $\sum_{t=1}^{T} \alpha_t = 1$ thereby allowing each coefficient to be interpreted as a relative importance measure. The context vector is subsequently obtained through weighted feature aggregation.

$$C = \sum_{t=1}^{T} \alpha_t \, h_t \tag{48}$$

Condensed conductivity-aware vectors highlight extremely informative nanocomposite properties. A self-attention mechanism enhances feature interactions. The query, key, and value matrices are built.

$$Q = HW_Q, K = HW_K, V = HW_V \tag{49}$$

Where W_Q, W_K, W_V characterize trainable projection matrices. The self-attention scores are computed through scaled dot-product attention.

$$A = Softmax\left(\frac{QK^T}{\sqrt{d_k}}\right) \quad (50)$$

Where d_k signifies the key dimension. The enhanced conductivity representation becomes

$$Z_A = AV \quad (51)$$

This operation lets the model find hidden interactions between distant conductivity-related descriptors that convolutional or recurrent processes may miss. The final representation fuses context-aware and self-attention data.

$$F_{fusion} = \gamma C + (1 - \gamma)Z_A \quad (52)$$

Where $\gamma \in [0,1]$ controls the relative contribution of both attention mechanisms.

$$LN(x) = \frac{x-\mu}{\sqrt{\sigma^2+\epsilon}} \quad (53)$$

Where μ And σ^2 characterize feature mean and variance respectively. The normalized fused representation becomes

$$F^* = LN(F_{fusion}) \quad (54)$$

This conductivity-aware feature representation selectively weights filler dispersion, conductive channel creation, interfacial transport, and structural organization. Thus, the feature space is appropriate for ensemble meta-learning.

Ensemble Meta-Learning Optimization

Although deep neural networks excel in nonlinear modelling, their performance may differ among datasets due to initialisation, feature distributions, and training dynamics. Different learning techniques capture different material behaviour features in conductivity prediction challenges. Using a single predictor may limit robustness and generalisation.

The proposed HMEP-Net uses an ensemble meta-learning optimisation architecture with several predictive learners to tackle this difficulty. Individual models learn complimentary conductivity correlations, whereas a meta-learner predicts them together. Attention module-generated fused representation is

$$F^* = [f_1, f_2, \dots, f_m] \quad (55)$$

and serves as the input to multiple base learners. The first base learner corresponds to Extreme Gradient Boosting (XGBoost). Its prediction is characterized as

$$\hat{y}_1 = f_{XGB}(F^*) \quad (56)$$

The second learner utilizes Random Forest regression.

$$\hat{y}_2 = f_{RF}(F^*) \quad (57)$$

The third learner employs Support Vector Regression.

$$\hat{y}_3 = f_{SVR}(F^*) \quad (58)$$

The fourth learner corresponds to a fully connected deep neural regressor.

$$\hat{y}_4 = f_{DNN}(F^*) \quad (59)$$

$$M = [\hat{y}_1, \hat{y}_2, \hat{y}_3, \hat{y}_4] \quad (60)$$

A meta-learning layer then combines these predictions. The stacking representation is expressed as

$$S = W_m M + b_m \quad (61)$$

Where W_m denotes the meta-learner weight matrix. The ensemble prediction becomes

$$\hat{y}_{ens} = g(S) \tag{62}$$

Where $g(\cdot)$ characterizes a nonlinear activation function. To evaluate the reliability of individual learners, prediction uncertainty is estimated. The ensemble variance is computed as

$$Var_{ens} = \frac{1}{K}\sum_{i=1}^{K}(\hat{y}_i - \bar{y})^2 \tag{63}$$

Where K represents the sum of base learners and $\bar{y} = \frac{1}{K}\sum_{i=1}^{K}\hat{y}_i$ signifies the ensemble mean. Learners exhibiting lower prediction variance receive larger contribution weights. The adaptive ensemble weight is calculated as

$$w_i = \frac{1/Var_i}{\sum_{j=1}^{K} 1/Var_j} \tag{64}$$

subject to $\sum_{i=1}^{K} w_i = 1$. The final weighted ensemble prediction becomes

$$\hat{y}_{final} = \sum_{i=1}^{K} w_i\,\hat{y}_i \tag{65}$$

This adaptive weighting approach boosts resilience by highlighting dependable predictors and discouraging unstable learners. To use Bayesian hyper parameter adjustment to improve ensemble performance. Expression of optimisation objective

$$\theta^* = \arg\min_{\theta} L(\theta) \tag{66}$$

Where $L(\theta)$ shows validation error simultaneous thermal and electrical conductivity estimates, the ensemble output is the final feature representation.

Multi-Objective Thermal–Electrical Conductivity Prediction

The framework aims at predicting both the thermal and electrical conductivity concurrently. These characteristics are physically correlated via filler dispersion, conductive network formation, interface quality, and microstructural structure. But they have different transportation systems. Electrical conduction is a function of electron mobility and percolation paths. Heat transfer is a function of phonon transport .Modelling all reactions simultaneously while keeping their unique qualities requires a multi-objective learning technique. Let the final ensemble representation be denoted as $E = [e_1, e_2, \ldots, e_d]$. The thermal conductivity prediction branch is expressed as

$$\hat{k} = W_k E + b_k \tag{67}$$

Where $\hat{k}$ represents foretold thermal conductivity. Similarly, the electrical conductivity branch becomes

$$\hat{\sigma} = W_\sigma E + b_\sigma \tag{68}$$

Where $\hat{\sigma}$ represents predicted electrical conductivity. The combined forecast vector is

$$\hat{Y} = [\hat{k}, \hat{\sigma}] \tag{69}$$

For thermal conductivity estimation, the prediction error is intended using Mean Squared Error.

$$L_{thermal} = \frac{1}{N}\sum_{i=1}^{N}(k_i - \hat{k}_i)^2 \tag{70}$$

Where k_i characterizes experimentally measured thermal conductivity. Similarly, electrical conductivity error is defined as

$$L_{electrical} = \frac{1}{N}\sum_{i=1}^{N}(\sigma_i - \hat{\sigma}_i)^2 \tag{71}$$

To avert model over fitting, parameter regularization is introduced.

$$L_{reg} = \lambda \sum_{j=1}^{P} w_j^2 \tag{72}$$

The overall optimization objective becomes

$$L_{total} = \lambda_1 L_{thermal} + \lambda_2 L_{electrical} + \lambda_3 L_{reg} \tag{73}$$

Where $\lambda_1, \lambda_2, \lambda_3$ control the relative influence of each objective. The parameter optimization process follows

$$\Theta^{t+1} = \Theta^t - \eta \nabla_\Theta L_{total} \tag{74}$$

Where Θ characterizes all trainable parameters of HMEP-Net. To assess prediction quality, the coefficient of determination is computed as

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2} \tag{75}$$

Forecast error is additionally quantified using RMSE.

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2} \tag{76}$$

and Mean Absolute Error.

$$MAE = \frac{1}{N}\sum_{i=1}^{N} | y_i - \hat{y}_i | \tag{77}$$

The HMEP-Net provides a continuous end-to-end framework for predicting conductivity behaviour in functional polymer-based nanocomposites using physics-guided conductivity encoding, nonlinear feature compression, hybrid CNN–BiLSTM learning, attention-based feature fusion, adaptive ensemble optimisation, and multi-objective prediction. The framework captures complex nonlinear interactions in material descriptors and preserves physically significant heat and charge conduction transport properties.

RESULTS AND DISCUSSION

Polymer-based nanocomposites' thermal and electrical conductivity is predicted by the advanced computational architecture Hybrid Multi-Physics Ensemble Prediction Network (HMEP-Net). Prediction environments include physics-guided modelling, deep learning, attention mechanisms, and ensemble learning. Python, NumPy, Pandas, and Scikit-learn were used for data preparation, feature management, normalisation, feature selection, regression modelling, and performance evaluation. TensorFlow/Keras built the auto encoder, CNN-BiLSTM, and Attention Fusion modules [23]. Gradient-boosting-based learning and Bayesian hyper parameter tuning were done with Boost.

The system has seven interconnected stages: multi-source feature representation, physics-guided conductivity encoding, deep auto encoder-based feature compression, CNN-BiLSTM hybrid feature learning, attention-based feature fusion, ensemble meta-learning optimisation, and multi-objective conductivity prediction. Some of the main material descriptors are: the fraction of filler volume, nanoparticle size, filler shape, aspect ratio, matrix density, matrix thermal conductivity, filler thermal conductivity, operating temperature, processing pressure, relative humidity, surface functionalization coefficient, dispersion coefficient, and agglomeration index. The dispersion-related descriptors determine the spatial distribution and uniformity of nano-fillers inside the polymer matrix and that's why are mainly responsible for the formation of conductive network. Features that are measured experimentally and derived from physics taken together represent structural compositional processing, and environmental characteristics for conductivity prediction in a comprehensive manner. The final system predicts thermal and electrical conductivity while following physical transport pathways. Improved material property prediction, less experimental reliance, and faster design optimisation of advanced polymer nanocomposite materials are possible with this integrated software system.

This analysis employed polymer nanocomposite material records from experimental conductivity investigations [24] and material characterisation databases [25]. Polymer-based nanocomposites' thermal and electrical transport behaviour is affected by compositional, structural, processing, and environmental factors in each sample. Filler volume fraction, nanoparticle diameter, aspect ratio, material density, matrix thermal conductivity, filler thermal conductivity, matrix electrical conductivity, operating temperature, processing pressure, relative humidity, and surface functionalization coefficient are the main inputs. Thermal and electrical conductivity results from experiments are the main variables.

The dataset that has been put together covers various functional polymer nanocomposites as reported in publicly available material databases and experimental research. It includes different polymer matrices like epoxy polyethylene polypropylene, polyvinyl alcohol, polydimethylsiloxane, and other engineering thermoplastics together with diverse conductive nano-fillers like carbon nanotubes, graphene nanoplatelets, graphene oxide, carbon black, boron nitride, aluminum nitride, silicon carbide, and metallic nanoparticles. Besides, the dataset contains samples produced through various processing routes such as solution casting, melt blending, hot pressing, extrusion, and in-situ polymerization. This variety allows the proposed HMEP-Net setup to gain knowledge of the generalized relationships between different material systems rather than being limited to one polymer, filler combination only.

The dataset was thoroughly pre-processed before model building. To reduce scale differences across characteristics, all numerical features were standardised using z-score normalisation and missing values were imputed. Pairwise interaction features were then created to represent nonlinear filler-processing condition connections. Maxwell effective thermal conductivity theory, Kapitza resistance correction, and percolation-based electrical conductivity formulations were used to calculate physics-guided conductivity descriptors. The original dataset was enhanced with these physically significant attributes to indicate conductivity.

All seven steps of the proposed HMEP-Net system employed the processed dataset. Initially, the physics-guided encoding module received all features. After maintaining important conductivity information, the deep auto encoder reduced the high-dimensional feature space into a compact latent representation. The CNN-BiLSTM network extracted local and sequential dependencies from compressed features

Adaptive feature weights helped the attention module identify the most significant conductivity-related descriptors. The ensemble meta-learning step used optimised latent features to provide complementing predictions from XGBoost, Random Forest, Support Vector Regression, then Deep Neural Network predictors. These predictions were incorporated using adaptive weighting to estimate thermal and electrical conductivity accurately and robustly.

The HMEP-Net architecture was compared to seven popular learning methods for material property prediction. Linear Regression (LR), a traditional statistical baseline, Support Vector Regression (SVR), which handles nonlinear regression problems, Random Forest Regression (RF), an ensemble tree-based learning approach, XGBoost Regressor, a gradient boosting algorithm widely used for predictive analytics, Deep Neural Network (DNN), which represents fully connected deep learning architectures, and CNN-LSTM, which combines convolutions.

The proposed Hybrid Multi-Physics Ensemble Prediction Network (HMEP-Net) integrates physics-guided conductivity encoding, deep auto encoder-based feature compression, CNN-BiLSTM hybrid learning, attention-based feature fusion, and ensemble meta-learning to provide enhanced prediction accuracy for both thermal and electrical conductivity in functional polymer-based nanocomposites.

Table 1 presents the thermal conductivity prediction performance of the proposed HMEP-Net against seven benchmark machine learning and deep learning representations. The results demonstrate a progressive improvement from conventional statistical methods toward advanced hybrid learning architectures. Linear Regression achieved the lowest performance with an R^2 value of 0.901 due to its inability to model nonlinear relationships among nanocomposite descriptors. Deep learning [26] approaches such as CNN-LSTM and Attention-CNN-BiLSTM improved prediction accuracy by capturing complex feature interactions. However, the proposed HMEP-Net achieved the best overall presentation with the lowest MAE (0.041), RMSE (0.061), and MAPE (3.12%), while obtaining the highest R^2 value of 0.985. This improvement is attributed to the integration of physics-guided conductivity encoding, deep feature compression, attention-based feature fusion, and ensemble meta-learning. The model incorporates thermal transport pathways that conventional approaches cannot, improving prediction accuracy and robustness by directly including conductivity theories into feature learning.

Table 2 compares prediction models for electrical conductivity. Because electrical conductivity depends on percolation, conductive network creation, and nonlinear interactions between fillers and matrix materials, standard models perform poorly, like thermal conductivity prediction [27]. The suggested HMEP-Net has the highest prediction accuracy (R^2 = 0.983), lowest MAE (0.047), and RMSE (0.069). The significant performance boost over Linear Regression and Support Vector Regression suggests that statistical correlations cannot accurately predict electrical conductivity.

The CNN-BiLSTM component learns conductive pathway patterns, whereas the attention module prioritises charge transport aspects. Ensemble learning also reduces prediction uncertainty by combining learners' complementary skills. These results show that the proposed framework accurately simulates polymer-based nanocomposites' complicated electrical conductivity behaviour.

The proposed HMEP-Net architecture's component contributions are examined in Table 3. The results show that every module improves prediction. Removing the Physics Encoding module reduces thermal and electrical R^2 values to 0.958 and 0.952, respectively, highlighting the need of physical conductivity knowledge in feature learning [28]. auto encoder removal affects performance because redundant and noisy information remains in the feature space. Removing CNN-BiLSTM learning reduces the model's local and sequential feature interactions. The model loses its capacity to prioritise highly influential conductivity features without Attention Fusion, degrading it further. Remove Ensemble Learning and the decrease is greatest, indicating that numerous predictors promote robustness and generalisation. The whole HMEP-Net obtains the highest R^2 values of 0.985 and 0.983, proving the usefulness of combining all modules into a single framework.

Table 4 compares all competing models' computational needs. Simpler approaches like Linear Regression and Support Vector Regression have fewer parameters and shorter training times. These models are less predictive. Due to their bigger parameter ranges and feature extraction capabilities, deep learning systems increase computational complexity. HMEP-Net had the most parameters (1.63 longest to train (61.8 minutes).

Table 1. Thermal conductivity prediction performance comparison.

Method	MAE	RMSE	MAPE (%)	R^2
LR	0.114	0.152	8.97	0.901
SVR	0.093	0.124	7.36	0.926
RF	0.082	0.108	6.44	0.941
XGBoost	0.076	0.101	5.87	0.949
DNN	0.069	0.093	5.12	0.957
CNN-LSTM	0.061	0.084	4.71	0.966
Attention-CNN-BiLSTM	0.055	0.078	4.29	0.972
HMEP-Net	0.041	0.061	3.12	0.985

Table 2. Electrical conductivity prediction performance comparison.

Method	MAE	RMSE	MAPE (%)	R^2
LR	0.131	0.176	10.34	0.887
SVR	0.108	0.142	8.83	0.914
RF	0.094	0.126	7.67	0.931
XGBoost	0.087	0.118	7.05	0.939
DNN	0.081	0.109	6.48	0.948
CNN-LSTM	0.071	0.096	5.79	0.961
Attention-CNN-BiLSTM	0.064	0.088	5.11	0.969
HMEP-Net	**0.047**	**0.069**	**3.58**	**0.983**

Table 3. Ablation study of HMEP-net components.

Configuration	Thermal R^2	Electrical R^2
Without Physics Encoding	0.958	0.952
Without auto encoder	0.964	0.960
Without CNN-BiLSTM	0.968	0.964
Without Attention Fusion	0.972	0.969
Without Ensemble Learning	0.977	0.974
Full HMEP-Net	**0.985**	**0.983**

Table 4. Computational complexity analysis.

Method	Parameters	Training Time (min)	Inference Time (ms)
LR	4.2 K	3.4	1.2
SVR	8.7 K	8.1	2.6
RF	52 K	15.3	5.1
XGBoost	64 K	18.5	4.8
DNN	0.82 M	34.2	8.5
CNN-LSTM	1.14 M	48.1	10.7
Attention-CNN-BiLSTM	1.42 M	57.6	12.4
HMEP-Net	1.63 M	61.8	13.2

Table 5. Robustness under noise conditions.

Noise Level	Thermal R^2	Electrical R^2
0%	0.985	0.983
5%	0.982	0.980
10%	0.978	0.975
15%	0.972	0.969
20%	0.965	0.961

It is much higher prediction accuracy justifies the extra computing expense. The 13.2 millisecond inference time is sufficient for real-time prediction and deployment. These results show that the proposed framework strikes a good compromise between computational complexity and predictive performance, making it ideal for advanced material informatics applications value accuracy above computational cost [29].

The resilience of HMEP-Net under varied artificial noise levels is shown in Table 5. The study found that thermal conductivity prediction maintains a R^2 value of 0.965 with 20% noise input, whereas electrical conductivity prediction maintains 0.961. As data corruption increases, forecast accuracy decreases, proving the model is stable. This robustness comes from autoencoder-based feature compression, attention-guided feature selection, and ensemble learning. These approaches mitigate noisy readings while maintaining conductivity data. Thus, the suggested approach is

generalisable and reliable for practical material characterisation scenarios.

Filler volume fraction and network connection index are shown in Figure 2. The S-shaped tendency is typical of polymer nanocomposites' conductive network development. At low filler concentrations, conductive particles are segregated, limiting connection and conductivity. Due of interconnecting conductive channels, network connection increases rapidly as the filler fraction reaches 5–7%. At the percolation threshold, conductivity rises substantially. Most conductive channels have been developed beyond this level, therefore connection approaches saturation. The graphic supports the Physics-Guided Conductivity Encoding module's physical assumptions and shows how filler concentration affects conductivity. The trend also explains why filler percentage was most important in future feature analysis.

The suggested framework's attention-based feature importance analysis is shown in Figure 3. Filler Fraction has the largest attention weight, indicating its dominance in conductivity prediction. AR and TC Ratios substantially affect conductive network development and heat transfer efficiency, making them the second and third most critical variables. Charge transport and interfacial interactions are also affected by Electrical Conductivity Ratio and Surface Functionalization. Temperature, Pressure, and Humidity are less important because of their indirect impacts. Attention discovers physically important conductivity drivers rather than weighting all characteristics equally. This interpretability shows that the model learns scientifically significant correlations and reveals nanocomposite conductivity behaviour's major drivers [30].

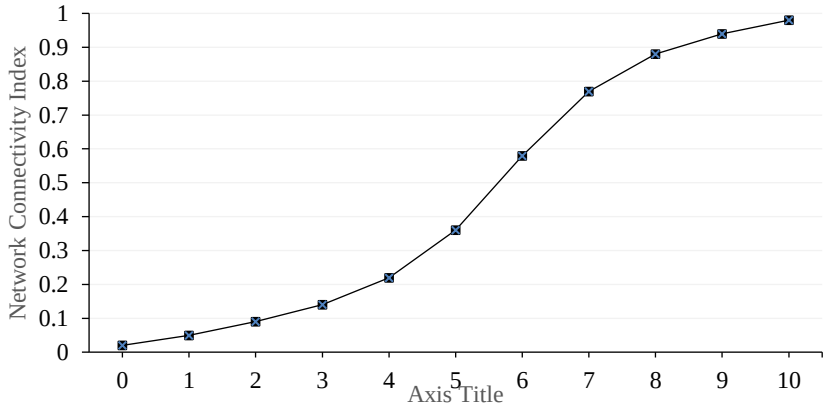

Figure 2. Conductive network evolution with increasing filler fraction.

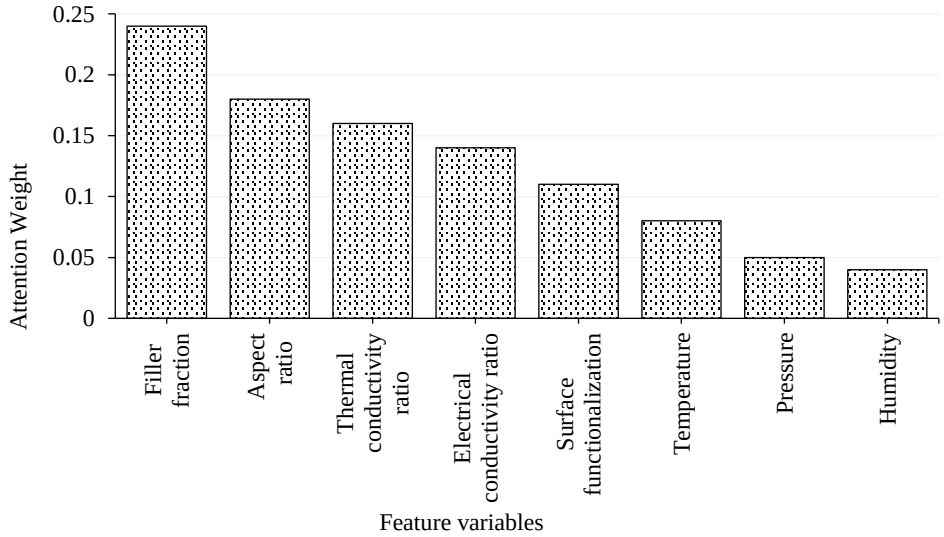

Figure 3. Feature importance ranking from attention module.

Figure 4 expressions HMEP-Net classical training optimisation. Convergence occurs when training and validation losses decrease continuously during learning. The close proximity of the two curves shows low over fitting and good generalisation. Because the network learns dominant conductivity patterns, loss lowers quickly in the early epochs. Improvement slows and stabilises at convergence throughout training. The optimisation procedure, residual learning connections, and attention-guided feature selection produce a smooth loss trajectory. Stable gradient propagation and effective parameter updates are confirmed by the absence of substantial oscillations. These findings confirm the framework's training stability then demonstration that it can learn complex conductivity correlations without optimisation issues.

Figure 5 demonstrations auto encoder compression then Attention-Based Feature Fusion latent features. Low, medium, and high conductivity clusters appear. Separating clusters reveals that the learnt feature space contains conductivity-related information and makes complicated material descriptors discriminative.

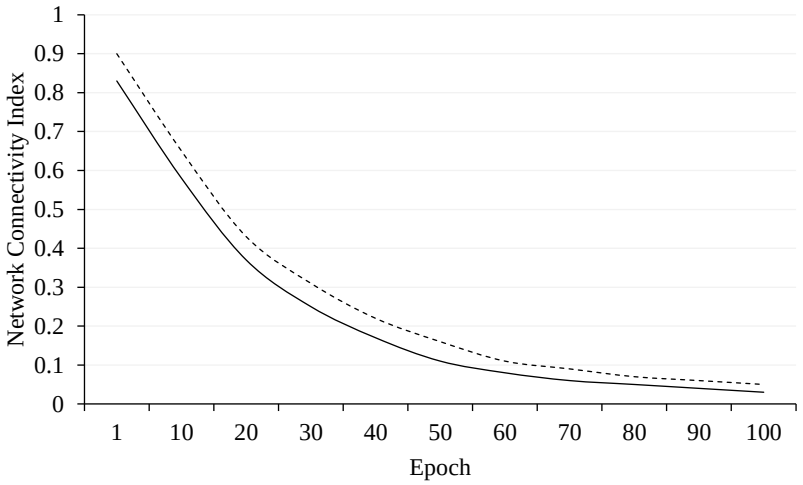

Figure 4. Training convergence of HMEP-net.

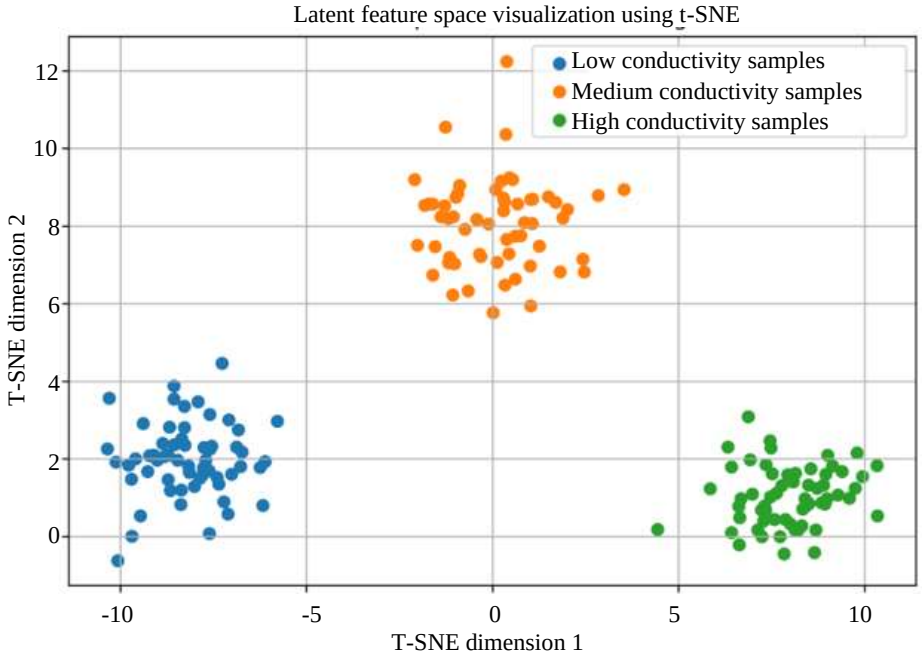

Figure 5. Latent feature space visualization using t-SNE.

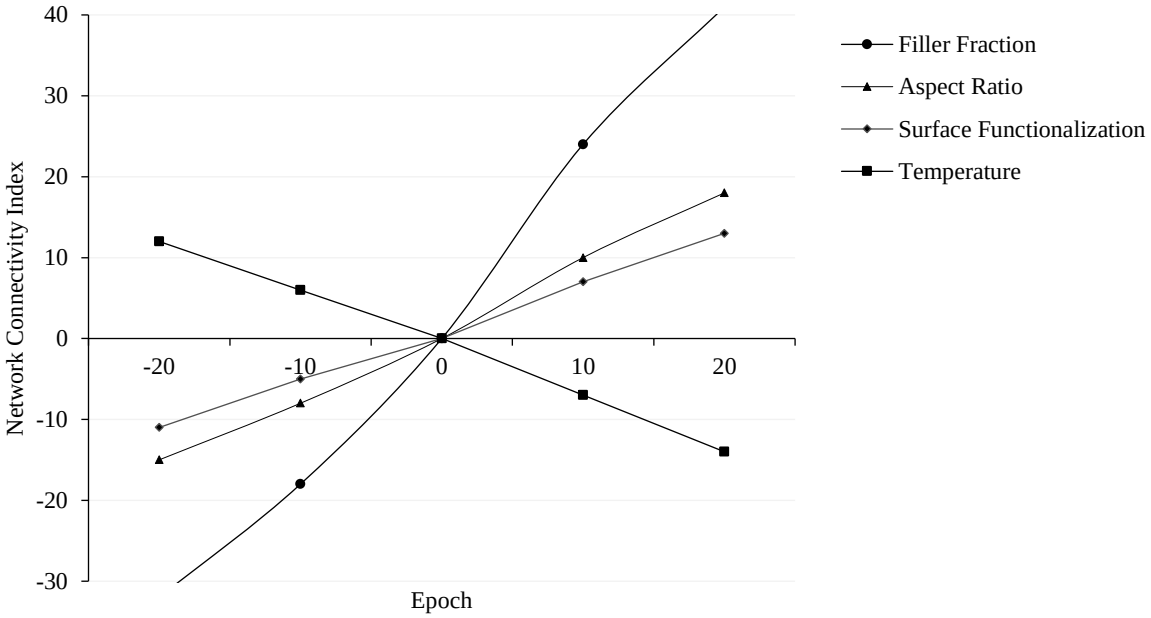

Figure 6. Sensitivity analysis of thermal and electrical conductivity.

The little cluster overlap suggests that feature extraction reduces conductivity category ambiguity. This illustrates auto encoder eliminates redundant information and attention mechanism accentuates conductivity features. HMEP-Net forecasts more correctly with well-structured latent space because cleanly separated feature clusters enhance regression and conductivity estimation.

Figure 6 primary input parameters affect conductivity predictions. Filler Fraction has the greatest impact on conductivity, causing the greatest positive and negative variations across the fluctuation range [31]. Elongated fillers create conductive pathways, making aspect ratio second significant. Surface functionalization moderately improves interfacial transport and filler dispersion. Temperature is inversely related to conductivity, demonstrating that thermal variations affect transport processes differently from structural characteristics. The sensitivity curve slopes reveal parameter influence and demonstrate model has learned significant conductivity correlations rather than statistical associations. These findings strengthen HMEP-Net outline's interpretability and physical consistency.

CONCLUSION AND FUTURE SCOPE

Physically consistent thermal and electrical conductivity predictions in functional polymer-based nanocomposites are made using HMEP-Net. Physical transport mechanisms and complex nonlinear relationships are captured using physics-guided conductivity encoding, deep auto encoder-based feature compression, CNN-BiLSTM hybrid learning, attention-based feature fusion, along with ensemble meta-learning optimisation on nanocomposite datasets. HMEP-Net outperformed seven benchmark approaches in both prediction tests. The model predicted heat conductivity with an MAE of 0.041, RMSE of 0.061, and R^2 of 0.985. The prediction of electrical conductivity got an MAE of 0.047, RMSE of 0.069, and R^2 of 0.983. Ablation analysis confirmed positive contributions from all architectural components, while robustness testing showed continuous performance up to 20% noise with R^2 values over 0.96. Filler %, aspect ratio, and conductivity ratios most affect transport behaviour, according to feature significance assessment.

The method might accelerate material discovery and minimise conductivity characterisation. HMEP-Net predicts characteristics fast and accurately for data-driven polymer nanocomposite formulation optimisation for energy storage, electronics, aerospace, biomedical, and multifunctional engineering applications.

Research may predict mechanical strength, thermal stability, dielectric behaviour, and corrosion resistance. Graph neural networks, transformer topologies, digital twins, and real-time production data may improve prediction accuracy and interpretability. Adding hybrid simulation-generated datasets to bigger experimental databases may increase generalisation and aid in developing intelligent material design systems.

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