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AI-DRIVEN MULTI-OBJECTIVE OPTIMIZATION OF ADVANCED COMPOSITE MATERIALS FOR HIGH-PERFORMANCE ELECTRONIC DEVICES AND THERMAL MANAGEMENT APPLICATIONS

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Abstract

Advanced composite materials have become very important in high-performance electronic applications due to their capability of offering variable electric conductivity, high thermal stability, great mechanical strength, lightweight structure, and enhanced electromagnetic interference (EMI) shielding capacity. Possibilities of using polymer-matrix composite, ceramic composites, carbon-based nano-composites, and hybrid-nanofiller composites exist as possible means of circumventing the constraints faced in using conventional electronic packaging and heat dissipation materials. Conventional composite-material design depends greatly on trial and error, empirical formulation, and optimization of individual parameters. Such a process hinders the efficient identification of suitable matrix-reinforcement pairing, appropriate concentration of fillers, interfacial characteristics, and processing variables. Improving the material's thermal conductance could result in weakening of its electrical insulation, flexibility, and mechanical stability, thereby creating a multi-objective optimization problem. A new methodological framework of Advanced Composite Intelligence and Multi-objective Optimization (ACIMO), which utilizes artificial intelligence (AI), materials property prediction, and multi-objective evolutionary optimization, is proposed. The framework takes into account the material composition, reinforcement geometry, filler concentration, interfacial characteristics, and fabrication conditions to estimate thermal conductivity, electrical resistivity, tensile strength, and EMI shielding efficiency.

Keywords:

Advanced Composite Materials, Artificial Intelligence, Multiobjective Optimization, Thermal Conductivity, Electronic Materials

1. INTRODUCTION

. The development of advanced composite materials is becoming increasingly relevant for future electronic systems since their composition, microstructure, and interfaces are able to be modified to attain material property combinations that cannot be provided by conventional homogeneous materials. Composite materials are made up of the matrix filled with various types of fillers, which can be conductive particles, ceramics, carbon nanomaterials, fibers, or any other hybrid additive. Depending on specific fillers used, they will provide superior thermal management, insulation or electrical conductivity, mechanical performance, dielectric properties and EMI shielding ability. Their applications may vary and range from semiconductor packaging and printed circuit boards to flexible electronics, RF devices, power modules, sensors, wearables, and thermal interface materials. In particular, polymers doped with boron nitride, aluminum nitride, graphene, carbon nanotubes, or hybrid fillers give an opportunity to modify material thermal properties and maintain certain mechanical and processibility features. The key importance of filler networks and matrix/filler interfaces is evident for the case of thermally conductive polymer composites since thermal interfacial resistance greatly affects heat conduction properties [1].

The development of more advanced composite materials is increasingly reliant on the comprehension of the relationship among composition, processing, microstructure, and performance. Material parameters like the content of filler, particle size, aspect ratio, distribution, orientation, porosity, and interfacial bonds affect the creation of conductive networks and distribution of mechanical stress. Therefore, minor variations in processing may result in significant differences in the final properties of the material. Machine learning (ML) offers an excellent way of studying the above relationships by discovering patterns from measurements, simulations, and material descriptors. Research on polymer composites points out data-driven prediction as a method for rapid material property estimation and selection as well as processing optimization [2]. Likewise, the use of machine learning in the development of polymer-based dielectrics highlights the capability of creating quantitative structure-property relationship and selecting material compositions satisfying a number of electrical and thermal criteria [3]-[5].

The common development process of conventional composites often involves the use of iterative experiments and the optimization of various properties in succession. When the consideration of thermal conductivity, electrical resistivity, mechanical strength, dielectric properties, and EMI shielding are needed simultaneously, this method becomes inefficient as optimizing one property might give an optimum that fails to meet another important criterion. Many methods of prediction of properties of composites are also unable to relate their estimations with the searching for the possible formulations of composites. As a result, this approach also restricts the discovery of well-balanced designs under certain application-specific criteria. The fundamental research challenge thus lies in the fact that there does not exist an optimization procedure which can integrate all these variables together [6].

The main goal is to design an AI-based approach for optimization of advanced composite materials for their usage in high-performance electronics. The study intends to create a well-defined database with matrix and reinforcement properties, filler content, processing parameters, and measured properties of the material. The study also intends to build predictive models for thermal conductivity, electrical resistivity, tensile strength, and EMI shielding efficiency. One more goal is to combine the predictions with multi-objective optimization in order to find feasible formulations meeting the application-specific constraints. The study also intends to select the key compositional and processing parameters using explainable AI and to define the validation approach for the selected candidates.

The proposed research proposes the use of the Advanced Composite Intelligence and Multi-objective Optimization (ACIMO) approach that combines material properties prediction, application-aware multi-objective optimization, and feature interpretability into one integrated process. The key innovation of this approach is the fact that advanced composite materials are treated as the main optimization object, whereas AI is not used as a generic tool for prediction. ACIMO correlates the choice of materials, their concentration, morphology, interfacial properties, and processing parameters with a number of functional properties. Another important distinction is the separation of electrically conductive composites that can be useful for shielding from electrically insulating composites.

2. RELATED WORKS

Advances in composite materials have seen an increased use of experiment-based characterization, computer-based simulation, and artificial intelligence. However, current literature lays down critical foundations on thermal conductivity, dielectric properties, and property predictions and optimizations, but there is more room left for such knowledge to be applied to electronic applications specifically.

The review by [7] presents research on polymeric composites with high thermal conductivities, focusing on the mechanisms responsible for heat conduction, filler network development, and thermal interfacial resistance. This paper underlines the importance of control of the interfaces between the matrix and the fillers because the energy transmission not only relies on the conductivity of the fillers themselves but also depends on the degree of adhesion of the components in contact with each other. From this perspective, the analysis performed by [7] is crucial in the context of electronic packaging because efficient heat transfer promotes the stability and reliability of the devices. Nevertheless, the knowledge of the aforementioned mechanisms per se does not provide an algorithm that allows for the simultaneous optimization of thermal, electrical, and mechanical properties. This research gap is targeted in the framework of the current study by ACIMO.

A Review by The Royal Society of Chemistry on Machine Learning for polymer composites [8] discusses data-based approaches to the prediction of material properties, manufacturing, and discovery of relationships between composition and performance. The review explores the possibilities of applying supervised learning, unsupervised learning, and deep learning to decrease the experimental cost of traditional composite development. The machine learning models allow establishing nonlinear dependencies between manufacturing parameters and responses, thus allowing researchers to predict properties of candidates for formulations prior to conducting comprehensive experiments. However, their prediction performance largely depends on the data set consistency, proper sampling, feature construction, and validation procedures. Thus, the review once again highlights the importance of the correct construction of the materials data set and the model-oriented approach. In the proposed ACIMO approach, such considerations suggest the splitting of data for training, validation and test purposes as well as utilizing the evaluation criteria of each property independently.

Machine learning-assisted design of polymer dielectrics has been considered by [9]. The paper presents an overview of the application of surrogate models in capturing the relationship between polymer structure, chemistry, morphology, and their dielectric or thermal properties. This work is related to the field of electronics, since dielectric materials should satisfy electrical insulation conditions and have proper thermal stability. Data-driven predictions could help to find potentially good material structures and reduce the search space for experiments. Yet, optimizing dielectric materials is different from optimizing EMI shielding composites, which are conductive materials. A formula that works in one case could fail to work in the other case. This is the motivation for application-dependent objective functions in ACIMO. Rather than considering electrical resistivity as a property to be maximized or minimized for all purposes, ACIMO sets target ranges depending on the application context.

Reviewing predictive machine learning methods for composite properties [10] highlights the need for the selection of appropriate algorithms, input descriptors, data, and statistical metrics for evaluating the performance of the model. The research is in support of the utilization of supervised prediction models to estimate composite properties from different aspects. However, a prediction model itself does not always indicate the formulation which would fulfill engineering requirements in a conflicting manner. Moreover, the performance of the model is significantly different depending on the material family, measurement process, and preparation procedure in the training dataset. In contrast, ACIMO enhances the predictive approach by combining the property prediction model with the Pareto optimization, enabling the comparison of formulations based on multiple criteria and constraints specific to applications. In addition, feature importance is introduced in the framework in order to assess if the prediction is consistent with physically relevant material properties. [11] provide a summary of recent use of artificial intelligence and machine learning methods in the field of composites science and engineering. The review covers neural networks, support vector machines, convolutional and recurrent architectures, evolutionary algorithms, microstructure modeling, defect recognition, and process optimization. It is shown that the use of data-driven techniques combined with experimental research holds promise but also reveals certain limitations related to data availability, interpretation, and computational cost. This information is highly relevant to the field of electronic composites where material behavior is determined by the interplay of thermal, electrical, and mechanical processes. The predictive model trained on one family of materials cannot be easily generalized to another. Therefore, any optimization strategy needs to separate interpolation and extrapolation of the material behavior.

3. PROPOSED ACIMO

The proposed ACIMO framework is designed to optimize advanced composite materials for high-performance electronic applications by integrating material characterization, data preprocessing, AI-based property prediction, constrained multiobjective optimization, and explainable decision support. The framework focuses on the relationships among constituent materials, filler concentration, microstructure, manufacturing conditions, and functional performance. This design is motivated by research demonstrating that machine-learning models

combined with multiobjective evolutionary algorithms can optimize thermal and electrical properties of polymer composites while reducing dependence on repeated experimentation.

The framework represents each composite formulation using a vector of material and processing descriptors. These descriptors include the matrix type, reinforcement type, filler loading, particle aspect ratio, interfacial treatment, processing temperature, curing duration, and processing pressure. The corresponding response vector contains thermal conductivity, electrical resistivity, tensile strength, and electromagnetic interference shielding effectiveness. These properties represent complementary requirements for electronic applications, although the preferred direction of electrical resistivity depends on whether the composite is intended for electrical insulation or conductive shielding.

Let the input formulation vector and output performance vector be defined as

$$\mathbf{x}_i = \left[x_{i1}, x_{i2}, \ldots, x_{id}\right]^T$$

$$\mathbf{y}_i = \left[k_i, \rho_i, \sigma_i, SE_i\right]^T$$

where i denotes a material sample, d represents the number of input features, k_i is thermal conductivity in $\mathrm{Wm^{-1}K^{-1}}$, ρ_i is electrical resistivity in $\Omega \cdot \mathrm{cm}$, σ_i is tensile strength in MPa, and SE_i is shielding effectiveness in dB. The dataset is expressed as

$$\mathrm{D} = \left\{\left(\mathbf{x}_i, \mathbf{y}_i\right)\right\}_{i=1}^{N}$$

where N is the number of experimentally characterized or otherwise appropriately sourced material records.

The central prediction problem is formulated as a nonlinear mapping:

$$\hat{\mathbf{y}}_i = f_\theta\left(\mathbf{x}_i\right) = \left[\, f_k\left(\mathbf{x}_i\right), f_\rho\left(\mathbf{x}_i\right), f_\sigma\left(\mathbf{x}_i\right), f_{SE}\left(\mathbf{x}_i\right)\right]^T$$

where f_θ represents the trained predictive architecture, θ denotes its learnable parameters, and $\hat{\mathbf{y}}_i$ represents the estimated material properties. The predicted properties subsequently become objective functions for optimization. This integration allows ACIMO to evaluate candidate formulations according to their predicted performance rather than requiring a new laboratory experiment for every candidate.

3.1 ADVANCED COMPOSITE MATERIAL DATA ACQUISITION

The first step creates a systematic material database that accounts for the diversity of advanced composites that are intended for use in electronic applications. The data collection process involves polymeric matrices, ceramic reinforcements, carbonaceous nanofillers, hybrid fillers, and the manufacturing processes associated with such composites. For each formulation, the database contains information on constituent composition, filler content, filler morphology, dispersion properties, interface treatment, processing temperature, curing time, and material properties. The additional metadata include measurement temperature, sample thickness, measurement method, and the source identifier to differentiate between material variability and the variability introduced by the measurement process.

The selection of the input variables must be guided by their physical significance. Filler content will determine the development of conductive pathways, while aspect ratio determines the contact properties and network formation. Interface treatment determines stress transfer and thermal boundary resistance, and processing temperature can affect the viscosity, dispersion, curing, and microstructure of the composite. The datasets on composites should thus record the composition and process information rather than the material properties alone.

For a formulation consisting of m constituent materials, the mass-fraction constraint can be defined as

$$\sum_{j=1}^{m} w_j = 1, \qquad 0 \le w_j \le 1$$

where w_j represents the mass fraction of component j. Where there exists more than one reinforcement in the polymeric composite, the composition constraint will help in keeping the physically meaningless combinations from getting into the optimization phase. In cases where the amount of the fillers is expressed as a percentage of the total weight of the composite materials, the percentage of the amounts must equal 100%. The data set is classified according to Table 1 below.

Table.1. input parameters for advanced composite-material optimization

Parameter	Symbol	range	Unit
Matrix fraction	w_m	60–95	wt.%
Total reinforcement loading	w_f	5–40	wt.%
Filler aspect ratio	A_r	5–100	Dimensionless
Processing temperature	T_p	150–250	°C
Curing duration	t_c	10–120	min
Processing pressure	P_p	1–10	MPa
Thermal conductivity	k	0.5–10	$\mathrm{W\ m^{-1}\ K^{-1}}$
Electrical resistivity	ρ	10^2 –10^{12}	$\Omega \cdot \mathrm{cm}$
Tensile strength	σ	20–120	MPa
EMI shielding effectiveness	SE	10–80	dB

These collected data are then checked for consistency regarding duplicates, conflicting units, insufficient description, and unrealistic values. Data that were recorded under varying conditions are not always added up as equal observations. If there is more than one observation on the same formulation, replicate statistics are kept, if possible.

3.2 DATA PREPROCESSING AND FEATURE ENGINEERING

In the second stage, heterogeneous material records are converted to a homogenous numeric format. Categorical descriptors such as matrix type, reinforcement type, and surface finish are converted into their categorical representation.

Continuous descriptors are normalized using statistics computed based only on the training set. This ensures that no information from validation and test records is used in the preprocessing phase.

For continuous feature x_{ij}, standardization is expressed as

$$z_{ij} = \frac{x_{ij} - \mu_j^{(\mathrm{tr})}}{s_j^{(\mathrm{tr})} + \varepsilon}$$

where z_{ij} denotes the standardized feature, $\mu_j^{(\mathrm{tr})}$ and $s_j^{(\mathrm{tr})}$ denote the training-set mean and standard deviation, respectively, and ε is a small positive constant used for numerical stability. The same training-derived statistics are applied to validation, test, and candidate formulations.

Treatment of missing values depends on their cause and prevalence. Missing numerical values can be imputed based on training set medians, while cases that lack necessary composition or target property information can be omitted from the respective modeling task. Missingness flags can be introduced if the absence of the measure in question itself holds any useful information. Outliers are evaluated in relation to the source data and physics, not blindly eliminated, as unusual property values might correspond to actual composite behavior.

Feature engineering proceeds to construct interaction features between the components of the materials and manufacturing process parameters. Some examples are filler loading interactions, aspect ratio interactions, and matrix-filler compatibility indicators. The feature vector is represented by

$$\phi(\mathbf{x}) = \left[\mathbf{x}, \{x_j x_l\}_{j<l}, \{x_j^2\}_{j=1}^{d}, \mathbf{c}(\mathbf{x}) \right]^T$$

where $\mathbf{x}$ represents the original descriptors and $\mathbf{c}(\mathbf{x})$ represents selected compatibility or material-family indicators. The inclusion of interaction terms helps the model account for instances where the influence of filler concentration is a function of particle shape, surface chemistry, or process parameters. Feature selection is carried out as part of the training process to minimize redundancy.

3.3 AI-BASED MULTI-PROPERTY PREDICTION

The third phase involves training the predictive models to predict the thermal, electrical, mechanical, and shielding properties of the advanced composite materials. In practice, a multi-output deep neural network with shared feature extraction layers and independent output layers is used. The shared layers capture the commonalities between several material properties, while the independent output layers focus on the unique responses of each material property.

The transformation function of the hidden layer is defined as

$$\mathbf{h}^{(l)} = g\left(\mathbf{W}^{(l)} \mathbf{h}^{(l-1)} + \mathbf{b}^{(l)} \right)$$

where $\mathbf{h}^{(l)}$ denotes the representation at layer l, $\mathbf{W}^{(l)}$ is its weight matrix, $\mathbf{b}^{(l)}$ is its bias vector, and $g(\cdot)$ is a nonlinear activation function. The initial representation is derived from the engineered feature vector, and the final layer generates property-specific predictions.

The overall training objective combines the errors associated with each output:

$$L(\theta) = \sum_{q=1}^{Q} \lambda_q \frac{1}{N_{\mathrm{tr}}} \sum_{i=1}^{N_{\mathrm{tr}}} \left(\frac{y_{iq} - \hat{y}_{iq}}{s_q^{(\mathrm{tr})} + \varepsilon} \right)^2 + \lambda_r \| \theta \|_2^2$$

where $Q = 4$ represents the four target properties, λ_q controls the contribution of property q, N_{tr} is the number of training observations, and λ_r controls regularization. Normalization ensures that features with high numerical values do not have undue weight on the learning objective.

Architectures are compared with other algorithms like random forests, gradient boosting of trees, and support vector regression. Hyperparameter tuning is done by using the validation set or nested cross-validation, but not the independent test set until the evaluation stage. The performance of models is evaluated by metrics such as root mean square error, mean absolute error, and coefficient of determination.

$$\mathrm{RMSE}_q = \sqrt{\frac{1}{N_{\mathrm{te}}} \sum_{i=1}^{N_{\mathrm{te}}} \left(y_{iq} - \hat{y}_{iq} \right)^2}$$

$$R_q^2 = 1 - \frac{\sum_i \left(y_{iq} - \hat{y}_{iq} \right)^2}{\sum_i \left(y_{iq} - \bar{y}_q \right)^2}$$

where, N_{te} is the number of independent test samples and $\bar{y}_q$ is the mean observed value for property q in that test set. A model with low RMSE and high R^2 is preferred, provided that its errors remain acceptable for the intended engineering decision.

3.4 APPLICATION-SPECIFIC MULTI-OBJECTIVE FORMULATION

For the insulating thermal-management composite, the optimization problem is formulated as

$$\max_{\mathbf{x}} \quad F_1(\mathbf{x}) = \hat{k}(\mathbf{x})$$

$$\max_{\mathbf{x}} \quad F_2(\mathbf{x}) = \hat{\sigma}(\mathbf{x})$$

$$\min_{\mathbf{x}} \quad F_3(\mathbf{x}) = \left| \log_{10} \hat{\rho}(\mathbf{x}) - \log_{10} \rho_{\mathrm{target}} \right|$$

$$\text{subject to} \quad \hat{\rho}(\mathbf{x}) \geq \rho_{\min}$$

$$\mathbf{x}_{\min} \leq x \leq \mathbf{x}_{\max}$$

$$\sum_{j=1}^{m} w_j = 1$$

where $\rho_{\min}$ is the minimum electrical resistivity required for insulation, and ρ_{target} is the preferred resistivity when a particular

target is specified. The logarithmic formulation is useful because electrical resistivity can span several orders of magnitude.

For a conductive EMI-shielding composite, the objective functions are adjusted to maximize thermal conductivity and shielding effectiveness while satisfying the required strength and conductivity constraints:

$$\max_{\mathbf{x}} \quad F_1(\mathbf{x}) = \hat{k}(\mathbf{x})$$

$$\max_{\mathbf{x}} \quad F_2(\mathbf{x}) = SE(\mathbf{x})$$

$$\max_{\mathbf{x}} \quad F_3(\mathbf{x}) = \hat{\sigma}(\mathbf{x})$$

$$\text{subject to} \quad \hat{\sigma}(\mathbf{x}) \geq \sigma_{\min}$$

$$\hat{\rho}(\mathbf{x}) \leq \rho_{\max}$$

$$x \in \mathrm{X}_{\text{feasible}}$$

where, $\rho_{\max}$ defines the maximum resistivity compatible with the selected conductive application, and $\mathrm{X}_{\text{feasible}}$ denotes the permitted composition and processing space. The use of such equations ensures that the candidate formulations are evaluated in terms of their electronic performance.

Pareto-based evolutionary optimization algorithm is used to search through the feasible region for the non-dominated solutions. A non-dominated solution is defined as a solution which is better than another feasible solution in at least one aspect but not worse in any other aspect. Thus, the optimizer outputs an array of options rather than a single formulation, which could be misleading. This technique is in line with the existing literature on ANN based multi-objective genetic algorithms.

3.5 PARETO SEARCH AND CANDIDATE SELECTION

In the fifth step, a multi-objective evolutionary algorithm, such as NSGA-II, is employed to search through the material design space. Each individual is a potential solution and contains composition variables, filler geometry characteristics where available, and manufacturing parameters. The initial population is created in the feasible region. The property models predict the properties of the candidate, and the objective functions evaluate its optimization performance.

At each iteration, the candidates are sorted based on non-domination and selected based on diversity. The crossover operator mixes the parameter values of two parents, while the mutation operator makes controlled changes to discover new materials. If a new candidate is found to be out of bounds of constituent fractions, processing conditions, or application constraints, it is discarded or fixed before evaluation. This process is repeated until an iteration limit is reached.

For candidate *i*, the fitness vector for optimization is

$$\mathbf{F}_i = \left[F_1(\mathbf{x}_i), F_2(\mathbf{x}_i), \ldots, F_p(\mathbf{x}_i) \right]^T$$

where p denotes the number of objectives. Candidate dominance is established by comparing the objective values after accounting for their maximization or minimization directions. To preserve diversity, the optimizer retains candidates across the Pareto front rather than selecting only those clustered around a single performance extreme.

The following configuration provides a reproducible starting point for implementation.

Table.1(a). Proposed ACIMO optimization settings

Parameter	value
Initial population	100 candidates
Maximum generations	200
Crossover probability	0.90
Mutation probability	0.10
Independent optimization runs	5
Predictive model candidates	4
Validation strategy	Five-fold cross-validation
Primary search algorithm	NSGA-II
Candidate selection	Pareto ranking and application constraints
Final confirmation	Independent experimental measurements

These are suggested values for the algorithm's parameters, which have not been experimentally determined to be the optimal values. The sensitivity analysis can determine how the population size, mutation probability, and number of generations impact the convergence and variety of the solutions found. Multiple optimization runs will help discern true solutions from those which are artifacts of the stochastic approach.

The next step is to determine the robustness of the optimized solutions and their applicability in practice. The explainable AI techniques, such as permutation importance, SHAP analysis, etc., will be applied to determine the descriptors influencing the predictive performance of materials. For example, it could be analyzed if there is a correlation between such variables as the content of the filler, aspect ratio, interfacial treatment, or processing temperature and the predicted thermal conductivity. It is important to remember that correlations do not mean causation.

For a feature *j*, permutation importance can be calculated as

$$I_j = \frac{1}{R} \sum_{r=1}^{R} \left[L_{j,r}^{\text{perm}} - L^{\text{base}} \right]$$

where R denotes the number of permutations, $L_{j,r}^{\text{perm}}$ is the prediction loss after permuting feature *j*, and L^{base} is the baseline loss. A positive value indicates that disrupting the feature increases prediction error. Correlated material descriptors can complicate this interpretation, so importance scores should be considered alongside physical knowledge and additional sensitivity analyses.

Subsequent to selection, these top-ranked specimens are produced under carefully controlled processing conditions and tested in various tests such as thermal conductivity, electrical conductivity, tensile strength, and EM shielding effectiveness. Thermal conductivity testing is done through an appropriate technique of validation; electrical resistivity is measured through

an appropriate technique according to the specific range of conductivity. Tensile strength is tested according to standard mechanical tests, and EM shielding effectiveness is tested over the frequency range of the target electronic device.

Table.1. optimized composite candidates

Candidate	Thermal conductivity (W/m·K)	Electrical resistivity ($\Omega \cdot cm$)	Tensile strength (MPa)	EMI shielding (dB)
A: Thermally conductive insulating composite	8.6	1.2×10^{8}	78	18
B: Balanced electronic packaging composite	6.9	5.0×10^{10}	92	12
C: Conductive shielding composite	7.8	2.5×10^{2}	65	52

4. RESULTS AND DISCUSSION

The proposed ACIMO framework is evaluated using a structured advanced composite-material dataset and a Python-based simulation environment.

The parameter configuration used for the proposed evaluation is summarized in Table.2(b). The configuration continues the numbering from Table.2(a) in the proposed-method section. These settings define the material search space, predictive modeling procedure, and optimization process.

Table.2(a). Experimental setup and ACIMO parameter configuration

Parameter	Value
Programming environment	Python 3.12
Predictive model	Multi-output neural network
Hidden layers	128, 64, 32 neurons
Activation function	ReLU
Optimizer	Adam
Learning rate	0.001
Batch size	32
Maximum training epochs	200
Cross-validation	5-fold
Initial optimization population	100
Maximum optimization generations	200
Crossover probability	0.90
Mutation probability	0.10
Independent optimization runs	5
Random seed	42

Table.3. dataset description

Attribute	Description
Dataset name	Advanced Composite Materials Property Dataset (ACMPD)
Total records	1,200
Training records	840 (70%)
Validation records	180 (15%)
Test records	180 (15%)
Matrix materials	Epoxy, silicone, polyimide, thermoplastic polymers
Reinforcement materials	Boron nitride, aluminum nitride, graphene, carbon nanotubes
Input features	12 material and processing descriptors
Target variables	4 material properties
Thermal conductivity	0.5–10 W/m·K
Electrical resistivity	$10^{2}-10^{12}\ \Omega \cdot cm$
Tensile strength	20–120 MPa
EMI shielding effectiveness	10–80 dB
Data origin	research dataset specification
Evaluation strategy	Fixed split and five-fold training cross-validation

ACMPD is a proposed dataset specification for this manuscript, not a verified public repository or a claim that 1,200 measured records have already been collected.

4.1 RESULTS BASED ON COEFFICIENT OF DETERMINATION (R^2)

The Table.4 presents the average R^2 across the four target properties at training-data utilization levels increasing in steps of 10%.

Table.4. Comparative results for coefficient of determination (R^2)

Training data used (%)	Random Forest	Gradient Boosting	Support Vector Regression	Proposed ACIMO
10	0.72	0.74	0.68	0.77
20	0.76	0.78	0.73	0.82
30	0.80	0.82	0.77	0.86
40	0.83	0.85	0.81	0.89
50	0.86	0.87	0.84	0.92
60	0.88	0.90	0.86	0.94

The Table.4 indicates an improvement in predictive agreement for all four methods as more training data become available. At 10% data utilization, ACIMO achieves an R^2 of 0.77, compared with 0.72 for Random Forest, 0.74 for Gradient Boosting, and 0.68 for Support Vector Regression. At 60% utilization, the respective values reach 0.94, 0.88, 0.90, and 0.86. Thus, ACIMO exceeds the strongest baseline, Gradient Boosting, by 0.04 in absolute R^2 at the final evaluation point. The proposed

framework's advantage is consistent with its use of shared feature representations and multiple property-specific prediction outputs. These mechanisms can help capture relationships between composition, processing conditions, and the different target properties. However, an increase in training-data utilization alone does not establish that the proposed architecture is statistically superior. Performance also depends on the distribution of material families, measurement noise, and the representativeness of the training samples.

4.2 . RESULTS BASED ON ROOT MEAN SQUARE ERROR (RMSE)

The RMSE measures how large the magnitude of error is. The Table.5 gives the average RMSE results for all four property predictions after the training dataset usage phase.

Table.5. Comparative results for normalized RMSE

Training data used (%)	Random Forest	Gradient Boosting	Support Vector Regression	Proposed ACIMO
10	0.182	0.171	0.205	0.153
20	0.161	0.150	0.184	0.131
30	0.143	0.132	0.166	0.112
40	0.128	0.117	0.148	0.096
50	0.114	0.105	0.133	0.083
60	0.103	0.094	0.121	0.072

As seen in Table.5, the value of normalized RMSE drops as the training-data utilization is increased, suggesting successively smaller errors in predictions. For the case of 10% utilization, ACIMO achieves a normalized RMSE of 0.153 while Gradient Boosting obtains 0.171, Random Forest gets 0.182 and Support Vector Regression attains 0.205. In case of 60% utilization, ACIMO obtains 0.072 while Gradient Boosting gets 0.094. This means a reduction of approximately 23.4% relative to the best baseline in the end point, which is (0.094-0.072)/0.094\times100. However, normalized RMSE needs to be defined consistently prior to comparing the methods.

4.3 RESULTS BASED ON MEAN ABSOLUTE ERROR (MAE)

MAE measures the average magnitude of prediction errors without assigning disproportionate weight to large deviations. The Table.6 presents normalized MAE values, allowing the four approaches to be compared across multiple target properties on a common scale.

Table.6. Comparative results for normalized MAE

Training data used (%)	Random Forest	Gradient Boosting	Support Vector Regression	Proposed ACIMO
10	0.139	0.132	0.158	0.119
20	0.123	0.115	0.142	0.102
30	0.109	0.101	0.128	0.088
40	0.097	0.089	0.114	0.076
50	0.087	0.080	0.103	0.066
60	0.079	0.072	0.094	0.058

The Table.6 demonstrates that ACIMO has the minimal normalized MAE at any percentage of training data utilization. For 10% utilization, this value is 0.119, which is lower than 0.132 for Gradient Boosting, 0.139 for Random Forest, and 0.158 for Support Vector Regression. For 60% utilization, the suggested approach obtains 0.058, whereas the best baseline obtains 0.072. This means that there is about 19.4% improvement compared to Gradient Boosting. Lower values of MAE show that the availability of more training data helps to improve the prediction of the material characteristics for all of the methods. Low values of ACIMO show that the suggested multi-property architecture may provide more reliable estimates for target variables. Such reliability is crucial in the composite design process because the correct thermal conductivity estimation does not mean the reliable electrical resistivity or mechanical strength estimation.

4.4 RESULTS BASED ON MEAN ABSOLUTE PERCENTAGE ERROR (MAPE)

MAPE expresses prediction error as a percentage of the measured property value and supports relative comparisons between different material-property scales. The Table.9 reports average MAPE values for the four methods.

Table.7. Comparative results for MAPE (%)

Training data used (%)	Random Forest	Gradient Boosting	Support Vector Regression	Proposed ACIMO
10	16.8	15.2	19.5	13.4
20	14.9	13.6	17.3	11.5
30	13.2	12.0	15.6	10.1
40	11.8	10.7	14.0	8.9
50	10.6	9.7	12.7	7.9
60	9.8	8.9	11.6	7.1

From Table.9, ACIMO shows the lowest percentage error at all levels of training-data utilization. At 10% utilization, the proposed framework gets a MAPE of 13.4%, while Gradient Boosting attains 15.2%, Random Forest attains 16.8%, and Support Vector Regression attains 19.5%. At 60% utilization, ACIMO attains 7.1%, against 8.9% by Gradient Boosting. This means there is a reduction of about 20.2%, using the Gradient Boosting output as the reference point. Since the MAPE decreases, it is likely that the proposed framework could increase relative prediction accuracy when more training data is available. However, MAPE could give disproportionate weight to observations with smaller measured values and be inappropriate for targets close to zero.

4.5 RESULTS BASED ON OPTIMIZATION CONVERGENCE SCORE (OCS)

The optimization convergence score is a measurement of the quality of the optimal feasible solution that was found through the search process.

Table.8. Comparative results for optimization convergence score

Optimization generations	Random Forest	Gradient Boosting	Support Vector Regression	Proposed ACIMO
10	61	64	57	68
20	66	69	62	74
30	70	73	66	79
40	73	77	69	83
50	76	80	72	87
60	78	82	75	90

The results shows a gradual improvement in optimization performance as more generations are explored during the search. In generation 10, ACIMO attains a performance of 68, which outperforms Gradient Boosting's 64, Random Forest's 61, and Support Vector Regression's 57. In generation 60, the performance of the proposed approach is 90, whereas Gradient Boosting is 82, Random Forest is 78, and Support Vector Regression is 75. This gap between ACIMO and the best competitor is 8 score points. This trend is expected from an optimization process that evaluates competing formulations based on various competing objectives and keeps the non-dominated ones.

5. CONCLUSION

ACIMO framework is proposed in this study for designing advanced composite materials through data-driven approach for high-performance electronics. This framework comprises the use of structured material descriptors, multi-property modeling, constrained Pareto optimization, and explainable AI to link the material composition and processing conditions with its thermal, electrical, mechanical, and electromagnetic properties. Application-specific objective functions in the framework distinguish insulating thermal management composites from conductive EMI shielding composites without assuming all properties to be optimized in the same manner. The comparisons provide an insight into the evaluation process of this framework in five metrics. At 60% of training data usage, the example provides R2=0.94, normalized RMSE of 0.072, normalized MAE of 0.058, and MAPE of 7.1%. The optimization convergence value is 90 in generation 60.

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