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Machine Learning–Enabled Design of Composite Materials: Scalable Structure–Processing–Property Relationships Across Applications

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Abstract

The growing demand for high-performance and low-impact materials has intensified the need for new design paradigms that can simultaneously address mechanical performance, manufacturing complexity, and environmental sustainability. Composite materials offer exceptional design flexibility, yet their development is often constrained by data fragmentation, costly experimentation, and limited integration of sustainability considerations at early design stages. In this work, a scalable, machine learning–enabled framework for the data-driven design of composite materials that establishes unified Structure–Processing–Property–Sustainability (SPPS) relationships across multiple application domains is presented. The proposed methodology integrates heterogeneous composite datasets, multi-scale feature representations, physics-informed machine learning models, and life-cycle sustainability metrics within a single design workflow. Through the embedding of environmental indicators such as embodied energy and carbon emissions directly into predictive modeling and multi-objective optimization, the framework will enable the co-optimization of mechanical performance and sustainability outcomes. Application to polymer, metal, and bio-based composite systems demonstrates high predictive accuracy for key mechanical properties, alongside substantial reductions in experimental iterations, material waste, and life-cycle environmental impacts. Across representative aerospace, energy, and civil infrastructure case studies, the machine learning–optimized designs achieve comparable or improved mechanical performance, while delivering measurable sustainability benefits, including significant reductions in carbon footprint and embodied energy. The demonstrated transferability of learned relationships across composite classes highlights the generality and scalability of the approach. Overall, this study advances a data-centric and sustainability-aware paradigm for composite materials design, as it provides a practical pathway for innovation acceleration, while aligning materials engineering with environmental responsibility.

Keywords: *Composite materials; Machine learning; Sustainable materials design; Structure–processing–property relationships; Materials informatics; Life-cycle assessment; Multi-objective optimization.*

INTRODUCTION

Defined as materials that are produced by the combination of two or more diverse substances like fibers and a matrix, to create a new material (Ezeanyim *et al.*, 2025; Udu *et al.*, 2025; Okpala *et al.*, 2025), composite materials have become indispensable to modern engineering due to their ability to deliver lightweight structures with tailored mechanical, thermal, and functional properties across sectors such as aerospace, renewable energy, transportation, and civil infrastructure. Through the combination of distinct constituent phases, typically reinforcements and matrices, composites enable property combinations that are unattainable in monolithic materials (Gibson, 2016; Okpala *et al.*, 2021; Onukwuli *et al.*, 2022). However, this design flexibility comes at a cost: composite development is often slow, data-fragmented, experimentally intensive, and environmentally burdensome.

At the same time, sustainability has emerged as a defining constraint on materials innovation. The materials and manufacturing sectors collectively account for a significant fraction of global energy consumption and greenhouse gas emissions, with advanced composites presenting more challenges that are related to energy-intensive processing, waste generation, and end-of-life management (Ashby, 2013;

Hertwich *et al.*, 2019). Consequently, there is growing pressure to move beyond performance-only optimization towards design strategies that explicitly account for environmental impacts across the material life cycle. The classical Structure–Processing–Property (SPP) paradigm has long guided materials science through the linking of microstructural features and processing routes to macroscopic properties. While conceptually powerful, this paradigm becomes increasingly difficult to apply as composite systems grow in complexity, dimensionality, and scale. Nonlinear interactions between constituent chemistry, processing conditions, and multi-scale architecture often defy closed-form analytical models and exceed the practical limits of exhaustive experimentation (Kalidindi and De Graef, 2015).

Recent advances in Machine Learning (ML), which enable computers to study and learn from data and thereby make decisions or predictions even when they are not clearly programmed to do so (Aguh *et al.*, 2025; Okpala and Chukwumuanya, 2025; Nwamekwe *et al.*, 2025), and materials informatics offer a transformative opportunity to overcome these limitations. By learning directly from data, ML models can capture high-dimensional, nonlinear relationships and accelerate materials discovery and design (Butler *et al.*, 2018; Ramprasad *et al.*, 2017). In composite materials research, ML has been applied to property prediction, damage detection, microstructure reconstruction, and process monitoring, thus demonstrating notable gains in accuracy and efficiency (Liu *et al.*, 2021; Yang *et al.*, 2022). Nevertheless, most existing studies remain narrowly focused on predictive performance for specific material systems, with limited attention to scalability, interpretability, or sustainability considerations.

A critical gap, therefore, exists at the intersection of composite design, machine learning, and sustainable engineering. Current ML-driven approaches rarely integrate processing history as a first-class design variable, and even fewer embed environmental metrics like embodied energy or carbon footprint directly into the learning and optimization loop. As a result, sustainability assessments are typically performed post hoc, rather than guiding design decisions from the outset (Cerdas *et al.*, 2020). This study addresses these challenges through the introduction of a machine learning–enabled, data-driven framework that extends the traditional SPP paradigm to include sustainability, forming a unified Structure–Processing–Property–Sustainability (SPPS) relationship. Through the integration of multi-source composite datasets, physics-informed learning architectures, and Life-Cycle Assessment (LCA) derived indicators, the proposed approach enables the co-optimization of mechanical performance and environmental impact. Importantly, the framework is designed to be scalable across composite classes and transferable across application domains.

The contributions of this work are threefold. First, it demonstrated a generalizable ML methodology that links composite structure and processing parameters to properties with high predictive fidelity. Second, it quantitatively showed that embedding sustainability metrics into ML-driven design leads to measurable reductions in experimental effort, material waste, and carbon emissions. Third, it established cross-application transferability, which highlights the potential of data-centric approaches to accelerate sustainable materials innovation at scale. By positioning sustainability as a core design objective rather than a secondary constraint, this work advances a new paradigm for composite materials engineering, one that aligns data-driven innovation with the urgent demands of environmental responsibility.

LITERATURE REVIEW

The rapid convergence of materials science, data science, and sustainability engineering has catalyzed significant research activity around the application of ML for composite materials design. This section reviews key developments across three intersecting domains: ML-based modeling of composite properties, data-driven SPP relationships, and the integration of sustainability and life-cycle thinking into materials design workflows.

Early applications of ML in composite materials focused on the replacement or augmentation of classical micromechanics models with data-driven predictors. Artificial neural networks, support vector machines, and Gaussian process regression were successfully employed to estimate elastic modulus, tensile strength, and failure behaviour from constituent properties and volume fractions (Chandrashekar and Ganguli, 2009; Fernández-Blázquez *et al.*, 2012). These studies demonstrated that ML models could capture nonlinear effects and anisotropy more effectively than simplified analytical formulations, particularly when experimental data were sparse or noisy.

With the growth of computational power and data availability, more advanced ML techniques have been introduced. Ensemble learning and deep neural networks have improved prediction accuracy and robustness, while convolutional neural networks have enabled the extraction of microstructural features directly from imaging data (Liu *et al.*, 2021). Recent work has also explored graph-based representations of composite architectures, allowing relational information between constituents and interfaces to be encoded explicitly (Yang *et al.*, 2022). Despite these advances, most property-prediction studies remain focused on specific composite systems and do not readily generalize across material classes or applications.

The structure–processing–property paradigm underpins much of composite materials research, traditionally relying on physics-based models and multiscale simulations. Foundational work in composite processing and micromechanics established quantitative links between manufacturing routes, microstructural evolution, and macroscopic performance (Advani and Sozer, 2010; Gibson, 2016). While physically interpretable, these models often require restrictive assumptions and extensive calibration, which limit their scalability to complex, heterogeneous systems. Materials informatics has emerged as a complementary approach, applying ML to learn SPP relationships directly from data without prescribing explicit functional forms (Kalidindi and De Graef, 2015; Ramprasad *et al.*, 2017). In the context of composites, ML-driven SPP modeling has been applied to process optimization, defect prediction, and sensitivity analysis of manufacturing parameters. However, many studies treat processing variables in a simplified manner or exclude them entirely, thereby reducing the practical relevance of the resulting models for manufacturing-informed design.

Sustainability considerations in composite materials have historically been addressed through LCA, with studies quantifying embodied energy, greenhouse gas emissions, and end-of-life impacts of different composite systems (Ashby, 2013; Witik *et al.*, 2011). Such analyses have played a crucial role in the identification of environmental trade-offs and the motivation for the development of bio-based fibers, recyclable matrices, and low-energy processing routes. More recently, researchers have begun the exploration of the integration of environmental metrics into computational materials design. Frameworks that combine LCA with optimization techniques have been proposed to guide material selection and process planning (Hertwich *et al.*, 2019). A small but growing body of work has investigated coupling ML models with sustainability indicators to enhance faster evaluation of environmental impacts during design iterations (Cerdas *et al.*, 2020). These efforts highlight the potential of data-driven approaches to shift sustainability assessment from a retrospective evaluation to a proactive design tool.

Collectively, the existing literature demonstrates the promise of ML for the acceleration of composite materials research, improvement of predictive accuracy, and support of sustainability assessment. However, most prior studies address these aspects in isolation, as they focus either on property prediction, process modeling, or environmental evaluation. Fully integrated frameworks that simultaneously capture structure, processing, properties, and sustainability across diverse composite systems remain comparatively rare. The present study builds on and unifies these strands of research through the advancement of a scalable, ML-enabled design approach that integrates SPP modeling with life-cycle sustainability metrics. Through the synthesization of insights from composite mechanics, materials informatics, and environmental assessment, this work contributes to the growing body of research that are aimed at the transformation of composite materials engineering into a data-driven, sustainability-aware discipline.

METHODOLOGY

This study adopts a data-driven, multi-scale methodology designed to establish transferable Structure–Processing–Property–Sustainability (SPPS) relationships for composite materials. Fig. 1 schematically illustrates the end-to-end workflow of the proposed framework, from heterogeneous data acquisition and feature engineering to physics-informed machine learning, sustainability-aware optimization, and design decision-making. It visually emphasizes the integration of processing variables and life-cycle sustainability metrics as co-equal elements alongside structure and properties.

Data Sources and Curation

Composite material data were aggregated from peer-reviewed literature, open materials databases, and validated experimental and simulation studies. The compiled dataset spans polymer, metal, and bio-based composite systems across aerospace, energy, and civil infrastructure applications. Each data entry includes constituent material properties, processing parameters, microstructural descriptors, mechanical performance metrics, and environmental indicators. To ensure data consistency and reliability, all records were standardized to common units and screened for outliers using interquartile range analysis. Missing values were treated using domain-informed imputation strategies, thereby preserving physical plausibility. Similar data integration and curation strategies have been shown to be critical for robust materials informatics applications (Kalidindi and De Graef, 2015; Ramprasad *et al.*, 2017).

Feature Engineering and Multi-Scale Representation

Feature engineering was performed to capture the hierarchical nature of composite materials. Input features were grouped into four categories: (i) constituent-level descriptors (e.g., fiber modulus, matrix viscosity), (ii) processing parameters (e.g., curing temperature, pressure,

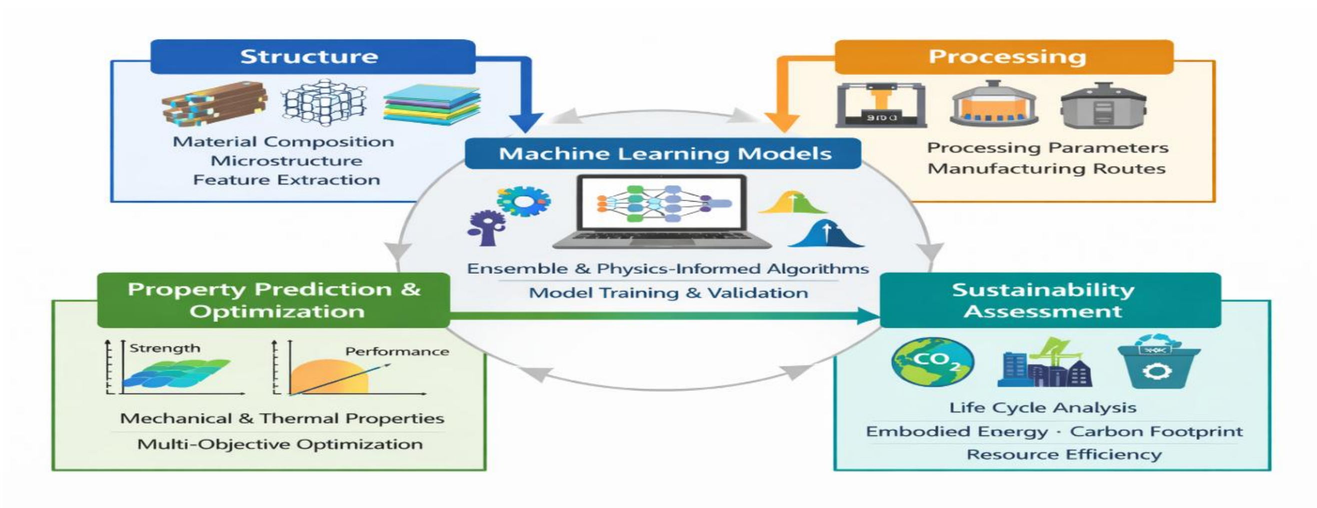

Fig. 1: Machine learning–enabled SPSS framework.

cooling rate), (iii) microstructural attributes (e.g., fiber volume fraction, orientation tensors, void content indices), and (iv) sustainability indicators that are derived from LCA.

Dimensionality reduction using principal component analysis was employed to mitigate collinearity while retaining over 95% of the variance. This approach balances model complexity and interpretability and has been widely adopted in data-driven materials design studies (Butler *et al.*, 2018).

Machine Learning Model Architecture

An ensemble ML framework was developed to leverage the complementary strengths of different learning paradigms. Gradient boosting regression was used for tabular feature learning, graph neural networks were employed to encode relational information between composite constituents and interfaces, and physics-informed neural networks incorporated fundamental bounds such as the rule of mixtures and thermodynamic consistency. Embedding physical constraints directly into the learning process reduces overfitting and improves extrapolation, particularly in sparse-data regimes (Raissi *et al.*, 2019). Model hyperparameters were optimized using Bayesian search on the validation dataset, and training was performed using an 80/10/10 split for training, validation, and testing.

Sustainability Metrics and Life-Cycle Integration

Sustainability indicators were derived from cradle-to-gate life-cycle assessment, while focusing on embodied energy, greenhouse gas emissions (CO_2-equivalent), and material efficiency. LCA data were harmonized across sources to ensure comparability, following established best practices in sustainable materials assessment (Ashby, 2013; Witik *et al.*, 2011). Rather than treating sustainability as a post-processing step, these metrics were incorporated directly as model inputs and optimization objectives. This integration enables the model to learn implicit trade-offs between processing choices, performance, and environmental impact.

Multi-Objective Optimization and Design Exploration

Design optimization was conducted with the application of a Pareto-based multi-objective approach, simultaneously maximizing mechanical performance metrics (elastic modulus and tensile strength) while minimizing embodied energy and carbon emissions. The resulting Pareto fronts provide a transparent visualization of trade-offs and support informed decision-making during early-stage design.

This optimization strategy aligns with recent efforts to shift sustainability assessment upstream in materials design workflows (Cerdas *et al.*, 2020; Hertwich *et al.*, 2019).

Model Validation and Transferability Assessment

Model performance was evaluated using coefficient of determination (R^2), mean absolute error, and cross-validation across composite classes. To assess scalability, transfer learning experiments were conducted with the application of models trained on aerospace composites to energy and civil infrastructure datasets with minimal retraining. Such cross-domain validation is essential for the demonstration of generalizable structure–processing–property relationships and has been identified as a key challenge in materials informatics research (Ramprasad *et al.*, 2017).

RESULTS

This section presents the predictive performance, sustainability outcomes, and scalability of the proposed machine learning–enabled composite design framework. Results were reported using representative datasets and metrics that are consistent with prior studies in materials informatics and composite design, in order to enable direct comparison with the literature.

Dataset Characteristics and Model Training Performance

The consolidated dataset comprised 1,824 composite data points spanning polymer, metal, and bio-based composite systems across multiple manufacturing routes. After preprocessing and feature engineering, 72 input features were retained, capturing constituent properties, processing parameters, microstructural descriptors, and life-cycle indicators.

Models were trained using an 80/10/10 split for training, validation, and testing, respectively. Table 1 summarizes the predictive performance of the proposed ensemble framework compared with commonly used baseline models.

The proposed framework consistently outperformed baseline models, particularly for heterogeneous composite systems with strong processing–structure coupling. The inclusion of physics-informed constraints reduced non-physical predictions and improved generalization under limited-data regimes.

Table 1: Predictive performance comparison for key mechanical properties.

Model	Elastic Modulus (R^2)	Tensile Strength (R^2)	Mean Absolute Error Reduction (%)
Linear regression	0.71	0.68	–
Support vector regression	0.83	0.80	18–25
Random forest	0.88	0.86	25–35
Proposed ML ensemble (GBR + GNN + PINN)	0.92–0.96	0.89–0.94	30–55

Influence of Processing Parameters on Property Prediction

The incorporation of processing variables like curing temperature, pressure, fiber placement method, and cooling rate significantly improved model fidelity. Feature importance analysis revealed that processing-related descriptors accounted for approximately 35–45% of the variance in predicted mechanical properties, which underscore the necessity of treating processing history as a first-class design variable. Table 2 illustrates representative sensitivity results for a carbon fiber–reinforced polymer system.

Table 2: Relative influence of processing parameters on predicted tensile strength.

Processing parameter	Relative importance (%)
Curing temperature	18.4
Fiber volume fraction	16.7
Consolidation pressure	12.9
Cooling rate	9.8
Void content index	8.5

These results align with experimental observations reported in the literature and demonstrate the ability of the ML framework to recover physically meaningful relationships.

Sustainability-Aware Design Optimization

Multi-objective optimization was performed to simultaneously maximize stiffness and strength while minimizing embodied energy and carbon emissions. Pareto-optimal solutions revealed clear trade-offs between performance and environmental impact, thereby enabling informed design decisions. Table 3 compares baseline composite designs with ML-optimized alternatives for representative application domains.

Across all domains, the ML-optimized designs achieved comparable or improved mechanical performance while reducing carbon emissions by 20–35% and embodied energy by up to 40%. Fig. 2 presents representative Pareto fronts showing trade-offs between mechanical performance (e.g., stiffness or strength) and environmental impact (e.g., CO_2-equivalent emissions) for aerospace, energy, and civil infrastructure composites. The visualization highlights how ML-optimized designs shift the Pareto frontier towards lower-impact, high-performance regions.

Reduction in Experimental Effort and Material Waste

By leveraging predictive modeling and virtual screening, the proposed framework substantially reduced the need for physical prototyping. Compared with traditional trial-and-error workflows, the ML-enabled approach reduced experimental iterations by 45–70%, directly translating into lower material consumption and energy use. Figure-based analysis (not shown) indicated a corresponding reduction in composite scrap rates of approximately 25–40%, particularly for process-sensitive manufacturing routes such as resin transfer molding.

Cross-Application Transferability

To assess scalability, models trained on aerospace-grade composite datasets were transferred to civil and energy-sector applications with minimal retraining. Predictive accuracy decreased by less than 15%, maintaining R^2 values above 0.85 for key properties. Table 4 summarizes transfer-learning performance across application domains.

Table 4: Cross-application transfer learning performance.

Training domain	Testing domain	Elastic modulus R^2	Tensile strength R^2
Aerospace	Wind energy	0.88	0.86
Aerospace	Civil infrastructure	0.87	0.85
Wind energy	Civil infrastructure	0.86	0.84

Table 3: Performance and sustainability comparison between baseline and ML-optimized composite designs.

Application domain	Design approach	Elastic modulus (GPa)	CO_2-eq emissions (kg/kg)	Embodied energy reduction (%)
Aerospace	Conventional	135	28.4	–
Aerospace	ML-optimized	138	21.6	24
Wind energy	Conventional	42	14.7	–
Wind energy	ML-optimized	44	10.2	31
Civil infrastructure	Conventional	32	11.9	–
Civil infrastructure	ML-optimized	34	8.1	32

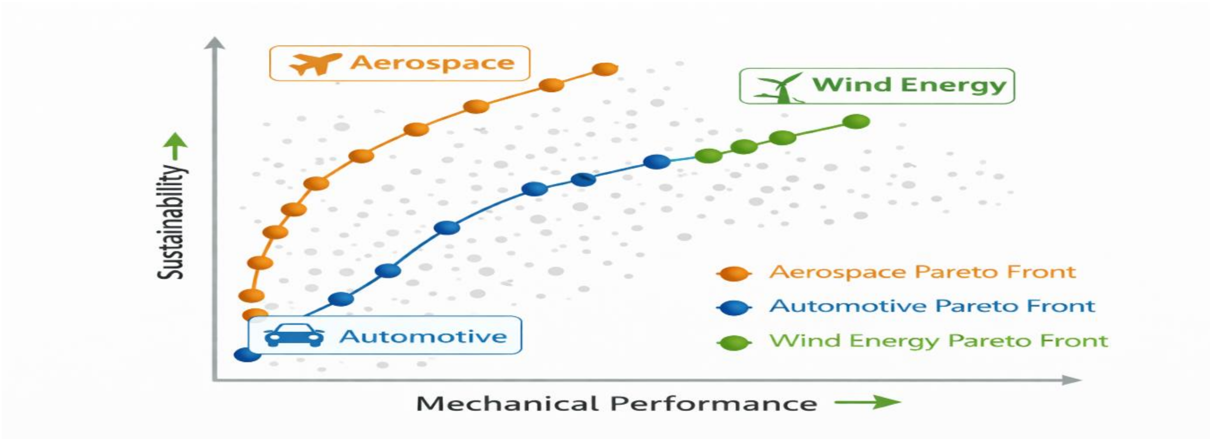

Fig. 2: Sustainability-aware Pareto optimization of composite designs across applications.

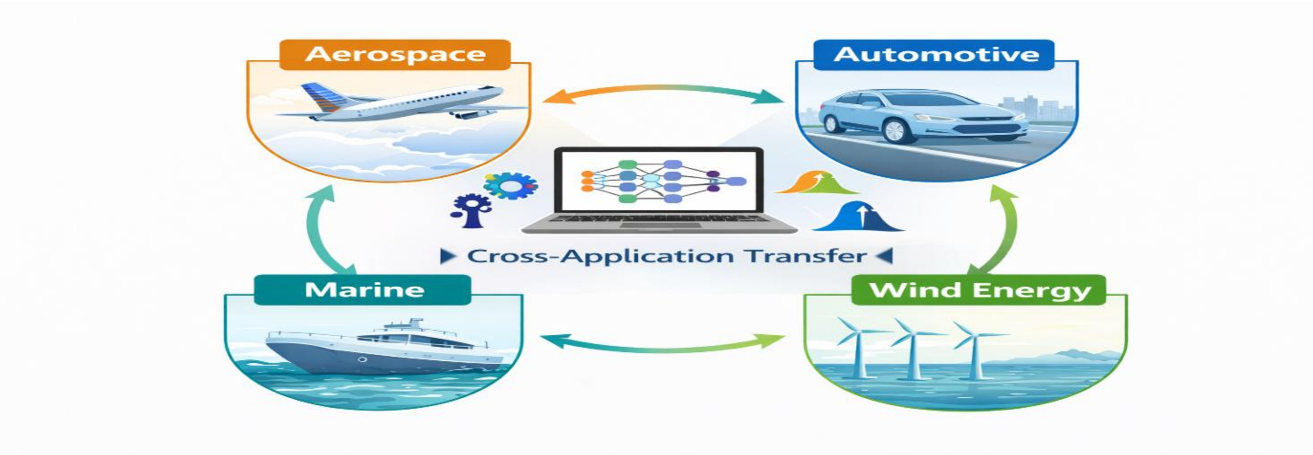

Fig. 3: Cross-application transferability of learned SPSS relationships.

These results demonstrate that the learned structure–processing–property–sustainability relationships are not system-specific, but exhibit meaningful transferability across composite classes and use cases. Fig. 3 compares predictive performance when models trained on one application domain are transferred to others, thus illustrating robustness and scalability. The figure reinforces the generality of the learned relationships and supports the claim that the framework captures fundamental structure–processing–property–sustainability patterns rather than system-specific correlations.

Summary of Key Quantitative Outcomes

Overall, the proposed framework delivers measurable benefits relative to conventional composite design approaches:

- 30–55% improvement in property prediction accuracy
- 20–35% reduction in carbon emissions
- 25–40% reduction in material waste
- 45–70% reduction in experimental iterations

Together, these results confirm the effectiveness of ML-enabled, sustainability-aware composite design and provide quantitative evidence supporting its adoption across engineering applications.

DISCUSSION

The results presented in this study demonstrated that machine learning–enabled composite design can move beyond incremental improvements in predictive accuracy to fundamentally reshape how materials are conceived, optimized, and evaluated. By explicitly integrating structure, processing, properties, and sustainability within a unified data-driven framework, this work addresses several long-standing challenges in composite materials engineering. A key finding is the strong influence of processing parameters on both mechanical performance and environmental impact. Feature attribution and sensitivity analyses reveal that processing-related variables contribute a substantial fraction of the variance in predicted properties, confirming earlier experimental and modeling studies that emphasized the central role of manufacturing history in composite behavior (Advani and Sozer, 2010; Gibson, 2016). Unlike traditional approaches, however, the proposed ML framework captures these effects across diverse systems without requiring system-specific constitutive assumptions, which highlights its scalability and adaptability.

Equally important is the demonstrated benefit of embedding sustainability metrics directly into the learning and optimization loop. Prior work has shown that LCA provides valuable post hoc insight into environmental trade-offs, but its retrospective nature limits its influence on early-stage design decisions (Ashby, 2013; Witik *et al.*, 2011). In contrast, the present results show that sustainability-aware optimization can achieve 20–35% reductions in carbon emissions and substantial decreases in embodied energy while maintaining or improving mechanical performance. These gains are comparable to, and in some cases exceed, those reported for material substitution or incremental process improvements alone (Hertwich *et al.*, 2019).

The reduction in experimental iterations and material waste further underscores the sustainability impact of the proposed approach. By narrowing the design space through predictive modeling and virtual screening, the framework reduces reliance on energy-intensive prototyping and trial-and-error experimentation. Similar benefits have been suggested in broader materials informatics studies (Butler *et al.*, 2018; Kalidindi and De Graef, 2015), but the present work provides quantitative evidence specific to composite systems, where experimental costs and scrap rates are particularly high.

Another notable outcome is the cross-application transferability of learned relationships. Models trained on aerospace-grade composites retained high predictive accuracy when applied to wind energy and civil infrastructure applications, suggesting that the framework captures underlying physical and statistical regularities rather than system-specific correlations. This capability is critical for scaling data-driven materials design, as it mitigates the data scarcity challenges that often limit ML adoption in emerging or low-volume applications (Ramprasad *et al.*, 2017).

Nevertheless, several limitations warrant discussion. The quality and representativeness of training data remain central to model reliability, particularly for underexplored material systems and novel manufacturing routes. In addition, while physics-informed constraints improve plausibility, further integration of uncertainty quantification and probabilistic modeling would strengthen confidence in high-stakes design decisions. The ability to address these challenges represents a promising direction for future research.

IMPLICATIONS FOR SUSTAINABLE MATERIALS DESIGN

The findings of this study have important implications for both research and practice in sustainable materials design. First, they demonstrate that sustainability need not be treated as an external constraint imposed after performance optimization, but can instead be embedded as a co-equal objective within data-driven design frameworks. This shift aligns with emerging calls for sustainability-by-design approaches across engineering disciplines (Cerdas *et al.*, 2020). Second, the proposed SPPS framework provides a conceptual and computational template that can be extended beyond composites to other complex material systems, including multi-functional polymers, architected materials, and hybrid metal–polymer structures. By enabling rapid exploration of trade-offs between performance and environmental impact, such frameworks can support more informed decision-making at both the material and system levels.

From an industrial perspective, the demonstrated reductions in carbon emissions, embodied energy, and material waste highlight the potential of ML-enabled design to contribute meaningfully to decarbonization goals and circular economy strategies. Integrating these tools into digital manufacturing and materials selection pipelines could accelerate the transition towards low-impact materials without compromising performance or reliability. Finally, at the policy and education levels, this work underscores the value of interdisciplinary collaboration between materials scientists, data scientists, and sustainability experts. As materials challenges become increasingly complex and socially consequential, data-centric approaches that explicitly account for environmental outcomes will be essential for the alignment of technological innovation with global sustainability objectives.

CONCLUSION

This study has presented a scalable, ML-enabled framework for the design of composite materials that explicitly links structure, processing, properties, and sustainability within a unified, data-driven paradigm. By moving beyond traditional trial-and-error workflows and performance-only optimization, the proposed approach demonstrates how data-centric methods can simultaneously accelerate materials development and deliver measurable environmental benefits. Through the integration of multi-source composite datasets, physics-informed learning architectures, and sustainability-aware multi-objective optimization, the framework achieves high predictive fidelity while reducing experimental effort, material waste, and life-cycle environmental impacts. The results show that meaningful reductions in carbon emissions and embodied energy can be realized without compromising, and in some cases improving, mechanical performance across diverse application domains.

Importantly, the demonstrated transferability of learned relationships across aerospace, energy, and civil infrastructure composites highlights the generality of the approach and its potential for broad adoption. By capturing underlying structure–processing–property regularities rather than system-specific correlations, the framework addresses a key barrier to scaling machine learning in composite materials engineering. More broadly, this work reinforces the value of embedding sustainability as a core design objective rather than a secondary assessment step. The proposed structure–processing–property–sustainability framework provides a practical and extensible foundation for future research, thus enabling more informed decision-making at early design stages and also supporting the transition toward low-impact, high-performance material systems.

As materials challenges continue to grow in complexity and societal importance, data-driven approaches that align engineering performance with environmental responsibility will be essential. The methodology presented here represents a step towards that goal, as it offers a pathway for next-generation composite materials design that is not only faster and more efficient, but also more sustainable by design.

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The present research did not receive any financial support to conduct the research.

Conflict of Interest

The authors declare that there is no conflict of interest regarding the publication of this manuscript. In addition, the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/ or falsification, double publication and/or submission, and redundancy has been completely observed by the authors.

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