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PERSPECTIVE ARTICLE

Physics-informed machine learning for material characterization: A perspective on data-efficient discovery through physics-informed neural networks

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Abstract

Accurate characterization of material properties is critical for modeling and optimizing advanced systems, yet conventional experimental and simulation-based approaches remain costly and data-intensive. As artificial intelligence evolves from data-driven modeling to physics-informed and knowledge-guided paradigms, this perspective article highlights the role of physics-informed machine learning (PIML), specifically physics-informed neural networks (PINNs), as a key enabler of data-efficient, physically consistent inference. PINNs embed governing equations into the learning process and have demonstrated strong capability in recovering constitutive and transport parameters from sparse or noisy data while preserving physical fidelity. This paper examines the fundamental structure, workflow integration, and recent advances of PINNs in the context of inverse material characterization. It also discusses open challenges in computational cost, training stability, and uncertainty quantification. Looking forward, integration with digital twins, generative modeling, and autonomous experimentation presents a pathway toward interpretable, adaptive, and automated characterization for next-generation intelligent manufacturing.

Keywords: Physics-informed neural network; Deep learning; Material property characterization; Physical AI

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1. Introduction

The rapid advancement of artificial intelligence (AI) and machine learning (ML) has profoundly transformed modern engineering. A clear trajectory has emerged toward knowledge-guided AI, where learning is informed not only by data but also by embedded physical principles and domain expertise.[1] The early phase of AI integration was largely driven by data-driven surrogate modeling, where large datasets were used to approximate complex physical responses without explicitly incorporating physical laws.[2-6] This paradigm has evolved toward generative modeling, where models approximate the data distribution and draw novel, distribution-consistent samples rather than memorized replicas of the training data.[7,8] It has further advanced toward physics-informed ML (PIML), which integrates governing equations and physical constraints directly into the learning process.[9,10] Most recently, the emergence of large

language models (LLMs) and agentic AI systems has accelerated this transformation, introducing autonomous reasoning, adaptive model construction, and closed-loop experimentation into engineering workflows,[11-13] as summarized in Table 1. Within this overarching framework of knowledge-guided AI, this perspective article represents the physics-knowledge-guided component, focusing on the physics-informed foundation through PIML and its core formulation, physics-informed neural networks (PINNs). As summarized in Figure 1, PIML encompasses several frameworks, including feature-augmented models, invariant and equivariant networks, PINNs, and operator learning methods.[9,14,15] Among these, this paper focuses on PINNs as a representative and widely adopted formulation that enables data-efficient, interpretable, and reliable characterization of material properties.

Such knowledge-guided transformation is particularly evident in material property characterization, where purely data-driven approaches often fail to capture the underlying physics that govern complex material behavior. Accurately identifying material properties, therefore, remains a persistent challenge in materials engineering and computational mechanics. Conventional experimental and numerical approaches—such as mechanical testing, curve fitting, or inverse finite element analysis—often require extensive data, significant computational effort, and substantial domain expertise.[16,17] These limitations are further exacerbated for non-linear, anisotropic, or coupled multi-physics systems, where replicating realistic boundary and environmental conditions is inherently difficult and measurement data are often sparse or noisy. Although ML-based surrogates can accelerate parameter estimation, they generally depend on large datasets and often lose physical interpretability, leading to limited generalization.[18-20]

To address these challenges, PINNs combine governing physical laws with data-driven learning, enabling reliable parameter identification under sparse or uncertain measurements while maintaining physical consistency.[21-23] Importantly, PINNs occupy a unique position in material characterization because they not only reduce data dependence but also restore the physical structure that governs constitutive behavior—something neither traditional inverse methods nor purely data-driven models can achieve. We argue that such physics-knowledge integration represents a necessary shift for material characterization problems in which data scarcity and physical fidelity must be jointly satisfied. A central theme of this perspective article is that PINNs should be viewed not merely as another modeling technique but as a foundational framework that unifies experimental observations, constitutive behavior, and computational modeling through explicit and implicit physics embedding. By providing structured inductive biases that guide inference toward physically admissible solutions, PINNs offer a principled route to overcome ill-posedness and enhance generalization across nonlinear, anisotropic, and emerging multi-physics systems. We highlight how PINNs complement existing experimental, numerical, and machine-learning approaches while also serving as a conceptual basis for next-generation hybrid, uncertainty-aware, and autonomous characterization pipelines. The remainder of this article outlines the PINN framework for material property identification and discusses representative applications, outstanding methodological challenges, and future opportunities for integrating PIML into digital-twin and intelligent manufacturing platforms.

2. Current status and challenges

This section supports our central argument by highlighting why traditional and data-driven approaches fall short and why physics-guided learning is needed. A critical challenge in material characterization is achieving reliable parameter identification under sparse, noisy, and often

Table 1. Summary of key AI paradigms, their implications, and limitations

Category	Representative models	Implications	Limitations
Data-driven surrogate modeling	GPR, CNN, LSTM	Accelerates surrogate modeling and design optimization	Strong data dependence; limited extrapolation
Generative AI	VAE, GAN, Diffusion models	Enables data augmentation and exploration of design spaces	Restricted by training distribution; no explicit physical constraints
PIML	PINNs, physics-informed neural operators, physics-constrained nets	Embeds governing equations to enhance data efficiency and physical consistency.	High computational cost
Agentic AI	LLM-based tool-using agents, multi-agent systems	Supports autonomous planning and knowledge-guided reasoning.	Complex implementation; limited real-time interpretability

Abbreviations: AI: Artificial intelligence; CNN: Convolutional neural network; GAN: Generative adversarial network; GPR: Gaussian process regression; LLM: Large language model; LSTM: Long short-term memory; PIML: Physics-informed machine learning; PINN: Physics-informed neural network; VAE: Variational autoencoder.

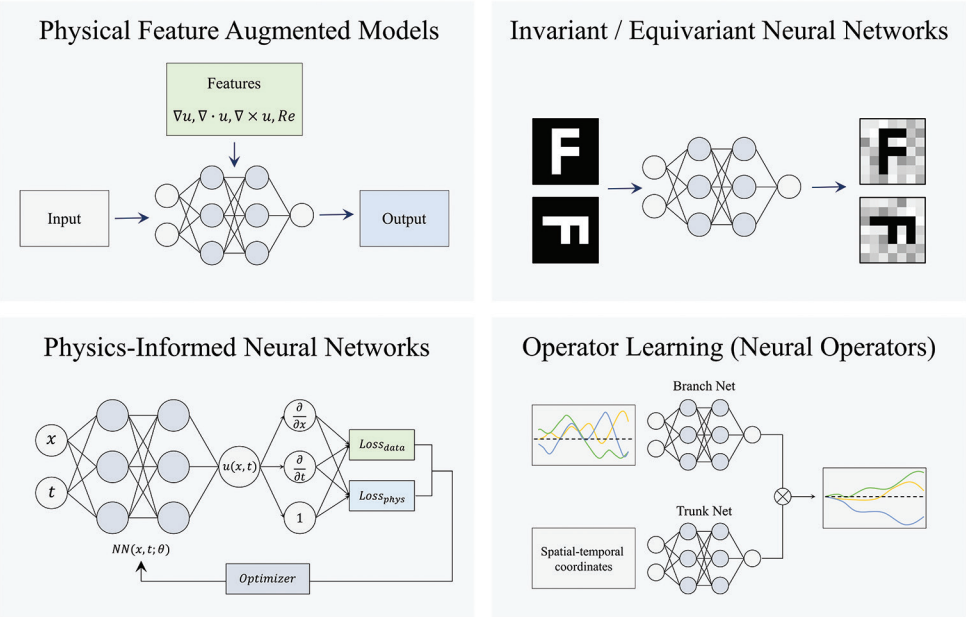

Figure 1. Four representative frameworks in physics-informed machine learning (PIML). Four representative frameworks of PIML are illustrated, including physical feature-augmented models that explicitly incorporate user-defined physical descriptors such as gradients or dimensionless numbers, invariant and equivariant networks that enforce physical symmetries through architectural design, physics-informed neural networks that embed governing equations into the loss function, and operator learning frameworks that learn mappings between function spaces. Image created by the authors.

costly measurements. Traditional inverse modeling approaches—such as curve fitting, finite element-based parameter optimization, and surrogate-assisted regression—have long supported the field, yet they remain limited by high computational cost, sensitivity to noise, and dependence on expert-driven trial-and-error procedures. These difficulties become more pronounced in nonlinear, anisotropic, or coupled multi-physics systems, where reproducing realistic loading and boundary conditions is inherently complex and experimental data are often sparse or uncertain.

In recent years, ML techniques have been explored as alternatives for accelerating material property identification. Methods such as neural networks, Gaussian process regression, and polynomial chaos expansion have been employed to correlate measured responses with underlying material parameters. These data-driven approaches can substantially reduce calibration time; however, their performance and generalization remain highly dependent on the quality and diversity of the available datasets. When data are limited, such models may suffer from overfitting and reduced generalization capability. Moreover, because physical constraints are often imposed externally rather than inherently embedded within the learning architecture, their interpretability and physical consistency can be difficult to maintain. On the other hand, physics-based inverse methods grounded in partial differential equation (PDE) formulations offer higher physical fidelity but remain computationally expensive and ill-posed, as multiple parameter sets can yield nearly identical responses. Even Bayesian inference, despite providing uncertainty quantification, can become computationally intractable for high-dimensional systems.

Building on these developments, PINNs have emerged as a promising hybrid paradigm that unifies data-driven learning and physics-based modeling. As illustrated in Figure 2, a PINN provides a unified framework applicable to both forward and inverse problems. In the forward setting, the network predicts physical field responses that satisfy governing equations for given material parameters and boundary conditions, whereas in the inverse setting, it identifies unknown material parameters from sparse or noisy measurements while preserving physical consistency. This bidirectional capability highlights the versatility of PINNs for integrating experimental data and physical modeling within a single learning architecture. Through this formulation, PINNs bridge the gap between conventional physics-based simulation and modern AI-driven discovery, laying the foundation for data-efficient and interpretable material characterization.

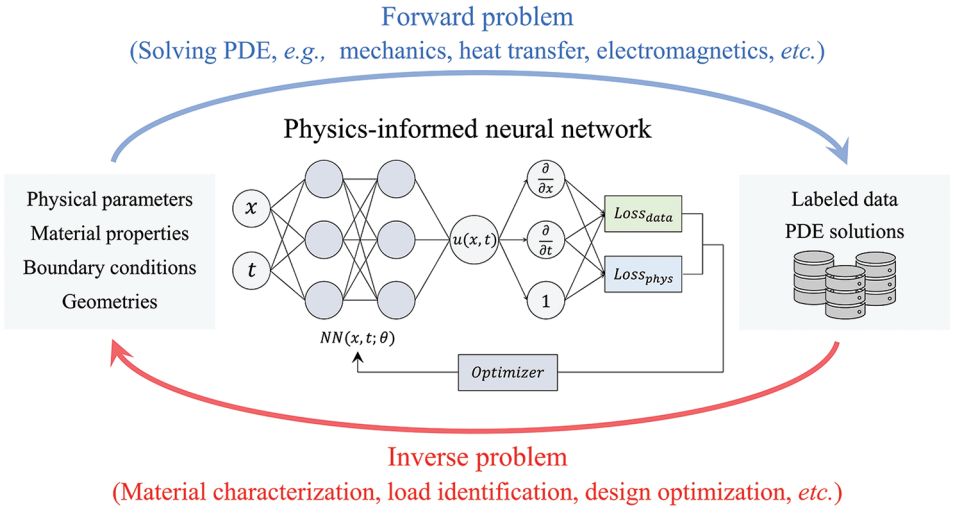

Figure 2. Schematic illustration of a physics-informed neural network (PINN) for forward and inverse problems. Image created by the authors. Abbreviation: PDE: Partial differential equation.

3. Opportunities of PINNs for material property characterization

A key claim of this perspective article is that PINNs uniquely bridge experimental data and governing physical laws, enabling material characterization approaches that remain reliable even under severe data scarcity. Rather than depending on large labeled datasets, PINNs embed the governing equations directly into the learning process, allowing the inference of material parameters and field quantities while maintaining physical consistency. By leveraging this physics-guided structure, PINNs mitigate overfitting and preserve admissible responses even when measurements are sparse or noisy, offering clear advantages over purely data-driven models. To better illustrate this concept, Figure 3 compares the conventional data-driven and physics-informed approaches for material property characterization. In the conventional approach, a neural network is trained on direct datasets such as stress–strain (σ, ε) pairs, which restricts its applicability to the training range and often results in non-physical extrapolation. In contrast, the physics-informed approach combines both direct and indirect data, such as displacement–force (u, F) measurements, with physical constraints and domain knowledge. By embedding this information into the training process, PINNs learn not only the mapping between inputs and outputs but also the underlying physical relationships. As shown in Figure 3, the conventional model fits the training data but diverges under unobserved conditions, whereas the physics-informed model maintains physically meaningful responses beyond the observed range. This capability makes PINNs particularly suitable for inverse material characterization, where experimental data are limited but the underlying physics is well established.

Beyond single-physics problems, the PINN framework can be readily extended to multi-physics systems such as thermo-mechanical, electro-mechanical, or flexoelectric materials by incorporating the corresponding governing equations into the physics-based loss term. This flexibility enables cross-domain inference, where different physical fields are coupled within a single learning framework. For instance, in thermoelectric systems, voltage measurements can be leveraged to infer thermal conductivity, enabling efficient estimation of transport properties without direct thermal measurements. Recent developments have further introduced Bayesian formulations of PINNs, which provide probabilistic uncertainty quantification and enhance robustness against sensor noise and incomplete data.[24] Such approaches extend the applicability of PINNs to real experimental settings while maintaining physical consistency and interpretability. Collectively, these capabilities position PINNs as a practical and robust tool for data-efficient, physics-consistent identification of material properties, bridging the gap between traditional inverse modeling and modern AI-driven materials design. The specific applications of this framework are discussed in Section 4.

4. PINN-based material characterization workflow

To illustrate how physics-informed learning can unify experiments, models, and simulations into a coherent characterization pipeline, this section outlines the integrated PINN-based workflow used in material

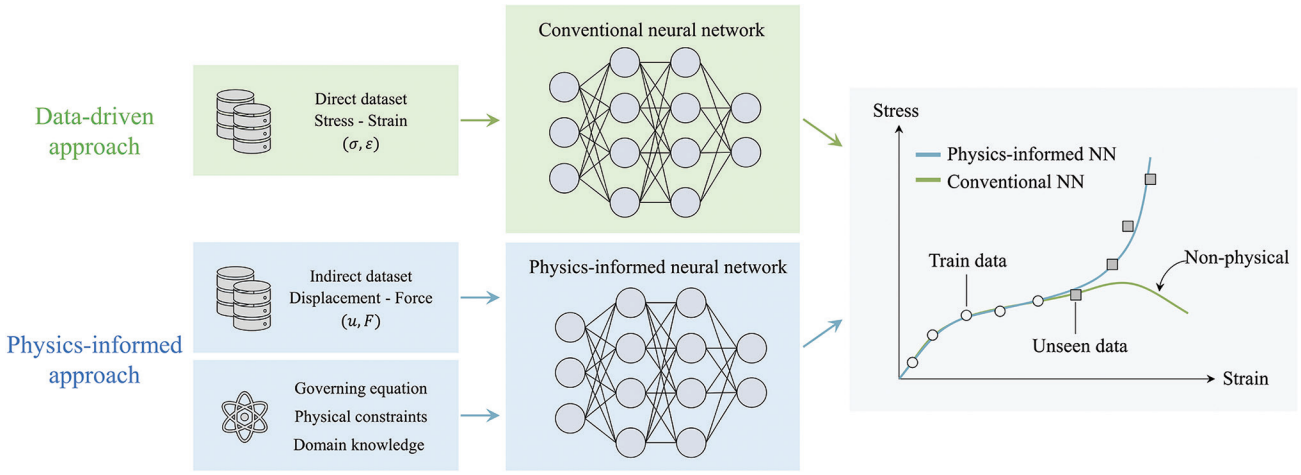

Figure 3. Comparison of conventional neural networks and physics-informed neural networks (PINNs) for material property characterization. Image created by the authors.
Abbreviations: NN: Neural network; PDE: Partial differential equation.

property identification. As illustrated in Figure 4, the workflow comprises five functional stages—data acquisition, dataset construction, constitutive modeling, PINN-based identification, and numerical validation—allowing physics-informed learning to bridge laboratory observations and computational mechanics in a coherent and data-efficient manner.

According to Figure 4, mechanical testing in stage (A) generates displacement, strain, or force data, which are organized in stage (B) into datasets that combine direct and indirect quantities for inference. Stage (C) introduces constitutive modeling, where analytical stress–strain relations may be replaced or augmented by neural representations whose parameters are treated as trainable variables. Stage (D) forms the core of the workflow: governing equations, boundary conditions, and measurement data are incorporated into a unified loss function that balances data fidelity with physical consistency. Different mathematical forms and training strategies may be used depending on the application, affecting computational cost without altering the underlying PINN formulation. Stage (E) then validates the inferred parameters or learned constitutive relations through finite element simulations or other high-fidelity solvers.

Although Figure 4 illustrates the workflow for mechanical characterization, the same structure extends naturally to thermal, electrical, thermoelectric, magneto-mechanical, and other coupled multi-physics systems through the incorporation of additional governing equations.[25-27] This generality underscores the role of PINNs as a versatile tool for physics-based characterization across diverse material classes. By unifying laboratory data, constitutive modeling, and computational verification in a single loop, PINNs provide the foundation for autonomous, closed-loop characterization pipelines central to digital-twin and AI-driven manufacturing systems.

5. Future directions and outlook

Looking ahead, establishing the foundations for reliable and widely adopted PINNs will require addressing several key challenges. The highest priority is establishing benchmark datasets that encompass diverse material systems, including elastic, thermal, electrical, and damage-sensitive materials, to ensure fair comparisons and reproducibility across studies. Equally important is integrating robust uncertainty quantification (UQ). Bayesian and probabilistic variants of PINNs provide a principled route to quantify predictive confidence and account for measurement noise, which is particularly important given the high sensitivity of inverse problems to sparse or biased data.[24,28-30]

Another major direction is improving the methodological scalability of PINNs for multi-scale and multi-physics systems. Although PINNs have shown strong potential in single-physics settings, extending them to coupled systems—such as thermo-mechanical or electro-chemical materials—remains challenging because multiple interacting field variables and complex constitutive couplings must be handled simultaneously. This gap highlights a notable opportunity for advancing data–physics fusion, where physics-informed learning could provide a unified representation across domains. Training such models, however, remains computationally demanding, particularly in high-dimensional or multi-physics settings where repeated differentiation of complex PDE operators amplifies the cost and causes instability

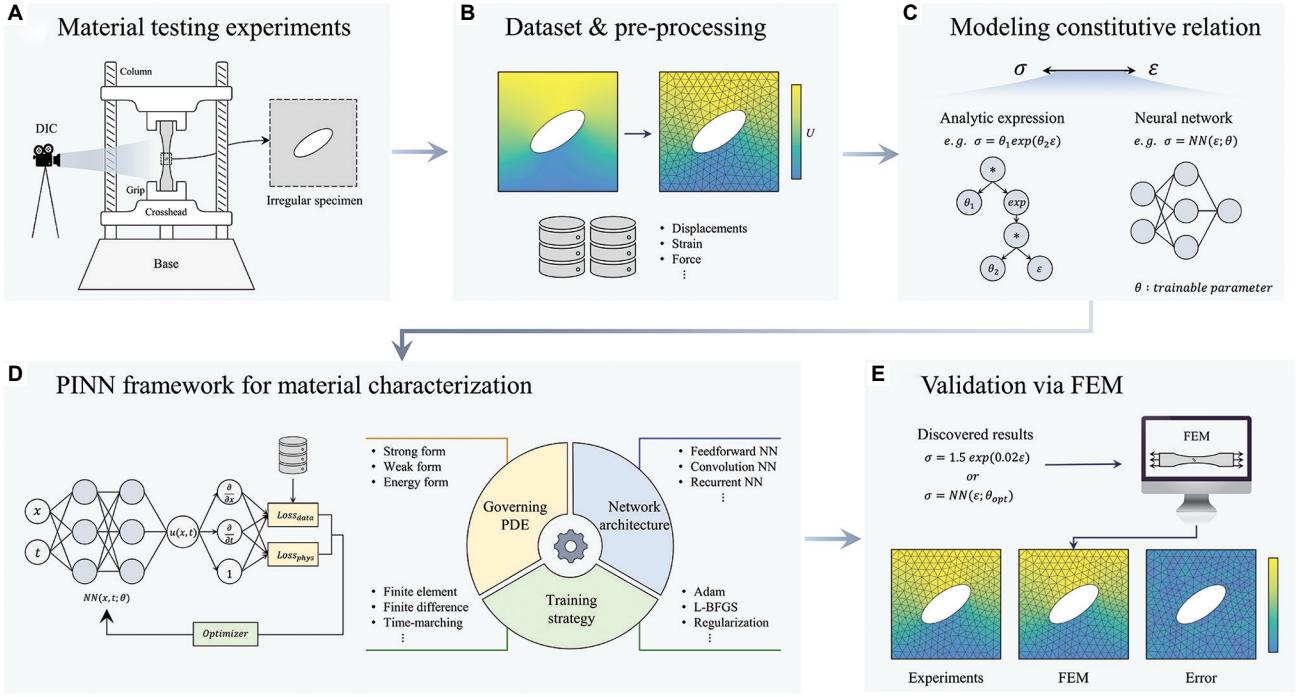

Figure 4. Representative workflow of physics-informed neural networks (PINNs) for material characterization. (A) Material testing and data acquisition; (B) Dataset construction and pre-processing; (C) Constitutive relation modeling; (D) PINN-based material characterization integrating governing equations, network architecture, and training strategy; (E) Validation via FEM simulations and experimental comparison. Image created by the authors. Abbreviations: FEM: Finite element method; L-BFGS: Limited-memory Broyden–Fletcher–Goldfarb–Shanno algorithm; NN: Neural network; PDE: Partial differential equation.

during optimization. Recent studies suggest that adaptive sampling, curriculum-based training, and operator-aware preconditioning can improve convergence stability, yet these techniques are not standardized and often require extensive problem-specific tuning.[31,32] In addition to computational cost, model-design decisions—including the choice of governing equations, network architectures, and loss formulations—remain highly problem-dependent and lack standardized best practices. A further challenge lies in extending PINNs to non-linear, history-dependent materials such as plasticity, viscoelasticity, and fracture, where internal state variables and path-dependent responses complicate learning.[33,34] Interpretability also remains limited, as the physical meaning encoded within learned latent representations is often unclear.

Finally, future material characterization pipelines are expected to evolve beyond classical PINNs toward hybrid, interpretable, and generative frameworks. Integrating generative modeling principles could alleviate the ill-posedness inherent in inverse problems, providing probabilistic descriptions of admissible material parameters rather than single deterministic estimates. Meanwhile, LLMs and knowledge-augmented networks may further enrich physical priors and assist in model design through embedded domain expertise.[35-37] In our view, achieving reliable, data-efficient, and autonomous material characterization will require models that not only learn from data and physics but also reason about uncertainty and adapt across material classes. Realizing this vision will establish PIML as a cornerstone of next-generation materials discovery and manufacturing.

From a broader perspective, we believe that advancing these directions will require closer collaboration across disciplinary boundaries. Experimentalists, computational mechanicians, materials scientists, and machine-learning researchers each contribute essential expertise—ranging from high-quality measurements and constitutive insight to scalable algorithms and physics-grounded architectures. Strengthening these connections will be crucial for translating physics-informed AI from promising methodologies into reliable, interpretable, and deployable tools for complex material systems. We view such interdisciplinary convergence as a necessary step toward building the next generation of characterization frameworks that seamlessly integrate data, physics, and intelligent automation.

6. Conclusion

The evolution of AI in materials science has advanced from purely data-driven modeling to generative, physics-

informed, and ultimately knowledge-guided paradigms. Within this progression, PINNs represent a pivotal step toward unifying data and physics for reliable and data-efficient material characterization. By embedding governing equations and physical constraints directly into the learning process, PINNs enable the inference of constitutive and material parameters even when experimental data are sparse, incomplete, or noisy. This integration of physical reasoning and ML has fundamentally reshaped the way materials are modeled, characterized, and designed.

Realizing the full potential of PIML, however, requires more than algorithmic innovation. The field must address challenges in data standardization, reproducibility, and computational scalability, while also developing robust frameworks for uncertainty quantification and interpretability. Collaborative efforts toward open benchmark datasets, standardized training protocols, and transparent evaluation metrics will be essential to ensure reliability and comparability across studies. Strengthening the integration between experimental and computational domains will further accelerate the transition from proof-of-concept demonstrations to practical engineering applications.

Looking forward, PIML is expected to evolve into hybrid and autonomous paradigms that combine the interpretability of physics with the adaptability of data-driven learning. Generative modeling principles, probabilistic inference, and knowledge-augmented architectures—potentially guided by LLMs—will further enhance physical understanding and enable intelligent design exploration. Ultimately, this convergence of physics, data, and intelligence is poised to transform materials research into a self-adaptive, closed-loop ecosystem capable of reasoning, learning, and discovery.

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Conflict of interest

Seunghwa Ryu serves as an Editorial Board Member of this journal, but was not in any way involved in the editorial and peer-review process conducted for this paper, directly or indirectly. Separately, other authors declared that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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Writing–review & editing: All authors

Ethics approval and consent to participate

Not applicable.

Consent for publication

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Availability of data

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