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Explainable AI for Interpretable Structure–Property Maps in Polymer Blend Systems

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Abstract

Polymer blend systems occupy a central position in soft matter materials science, where macroscopic properties emerge from complex, multi-scale interactions among molecular architecture, phase morphology, and processing history. Although artificial intelligence (AI) is increasingly used to predict properties of polymer blends, most existing approaches prioritize prediction accuracy over interpretability, limiting their contribution to theoretical understanding and rational materials design. This paper introduces a purely conceptual framework for explainable artificial intelligence (XAI)–enabled structure–property mapping in polymer blend systems, positioning interpretability as a foundational epistemic requirement rather than a post-hoc diagnostic. Given the recent advances in machine learning, polymer informatics, and explainable AI, the framework conceptualizes structure–property maps as interpretable landscapes where predictions, feature attributions, and uncertainty coexist as integrated elements. By explicitly incorporating multi-scale descriptors—from molecular chemistry to mesoscopic morphology—and embedding XAI mechanisms such as feature attribution and counterfactual reasoning, the proposed framework aligns data-based insights with established principles of soft matter physics and thermodynamics. Instead of advanced algorithms or empirical models, this work articulates a theoretical architecture that shows how AI-derived representations can support causal reasoning, trade-off analysis, and epistemic restraint in the design of the polymer blend. Ultimately, the paper provides a framework-level perspective on the application of AI in materials science and defends the structure–property mapping approaches, in which interpretability, physical grounding, and uncertainty awareness are central to scientific meaning and responsible materials innovation.

Keywords Artificial intelligence, Explainable AI, Structure–property maps, Polymer blends, Interpretable models, Soft matter

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Introduction

Polymer blend systems, comprising mixtures of two or more distinct polymers, constitute a paradigmatic example of soft matter in which emergent properties arise from complex interactions across length scales. These systems are ubiquitous in industrial applications, ranging from packaging films to automotive components, owing to their tunable mechanical, optical, and barrier properties [1-6]. At the core of their utility lies the structure–property relationship, which delineates how molecular architecture, phase separation dynamics, and interfacial phenomena dictate macroscopic performance [7]. For instance, the miscibility of the polymer components influences phase morphology, which, in turn, affects tensile modulus and impact resistance [8]. However, elucidating these relationships remains challenging due to the high-dimensional parameter space involving composition, molecular weight distributions, and processing conditions [9].

The advent of artificial intelligence (AI) has revolutionized materials science by enabling predictive modeling of complex systems without exhaustive experimentation [10]. In polymer blends, AI techniques have been employed to forecast phase behavior and property optima, leveraging large datasets derived from simulations or databases [11]. Recent studies highlight the efficacy of machine learning (ML) algorithms in capturing non-linear correlations that elude classical theories, such as the Flory-Huggins theory of thermodynamics [12]. For example, neural networks have demonstrated superior accuracy in predicting glass transition temperatures and solubility parameters in blended systems [13]. Yet, the "black-box" nature of many AI models poses a significant barrier to their adoption in theoretical materials research [14]. Without interpretability, these models offer predictions devoid of mechanistic insights, hindering the development of generalizable theories [15].

Explainable AI (XAI) emerges as a critical tool to address this opacity, providing methods to unpack model decisions and reveal underlying patterns [16]. In the context of materials science, XAI facilitates the translation of data-driven outputs into conceptually meaningful narratives, aligning with the field's emphasis on causal reasoning [17]. For polymer blends, interpretable structure–property maps could illuminate how specific structural motifs contribute to property enhancements, such as improved ductility through compatibilizer addition [18]. Literature from the specified period underscores the growing interest in XAI for soft matter, with applications in property prediction and inverse design [19]. However, existing frameworks often focus on singular properties or generic materials, neglecting the unique challenges of blend systems, including phase instability and multi-component interactions [20].

This gap is particularly evident in the synthesis of structure–property maps, which traditionally rely on empirical contour plots or phase diagrams that lack dynamic interpretability [21]. While AI can generate high-fidelity maps, the absence of explanation limits their utility for theoretical advancement [22]. For instance, gradient boosting models have mapped viscoelastic responses in blends, but without attribution to structural features, they fail to inform refinements in molecular design [23]. Moreover, the interdisciplinary nature of polymer science demands frameworks that integrate insights from chemistry, physics, and computation, yet current XAI applications in materials are fragmented [24].

The present manuscript advances a purely conceptual approach to this challenge by developing a novel theoretical framework for XAI-enabled, interpretable structure–property maps tailored to polymer blend systems. Grounded in soft matter principles, the framework posits a layered architecture that decomposes complex relationships into interpretable modules, fostering a deeper understanding of emergent behaviors [25]. By synthesizing recent literature, we identify key theoretical underpinnings and propose innovations that extend beyond existing models, such as incorporating uncertainty quantification for robust interpretations [26].

The introduction of this framework is timely, as the materials community increasingly recognizes the need for trustworthy AI [27]. In polymer blends, where sustainability drives the quest for bio-based or recyclable formulations, interpretable maps can guide the selection of compatible pairs, reducing trial-and-error [28]. Furthermore, this work aligns with broader trends in applied AI, emphasizing ethical and scientifically sound integration [29, 30].

Structurally, the manuscript proceeds as follows: The subsequent section provides a theoretical background and literature synthesis, delineating key concepts in structure–property relationships, ML in polymers, and XAI methodologies. We then articulate the proposed conceptual framework, detailing its components and logical flow. Future sections will outline propositions, discuss implications, and conclude with avenues for theoretical extension. Through this lens, we aim to contribute to the discourse on AI's role in advancing materials theory, particularly in soft matter domains.

Theoretical Background and Literature Synthesis

Structure–property relationships in polymer blend systems

Polymer blends represent a paradigmatic class of soft matter systems in which macroscopic properties emerge from a hierarchy of structural features spanning molecular, mesoscopic, and bulk length scales. The structure–property

relationships in such systems are governed by an interplay between thermodynamic driving forces, which dictate equilibrium phase behavior, and kinetic constraints, which arise during processing and often lock materials into non-equilibrium morphologies [6]. This dual control distinguishes polymer blends from small-molecule mixtures and renders their behavior particularly sensitive to processing history.

At the molecular level, chain architecture—including molecular weight distribution, tacticity, branching, and stiffness—plays a central role in determining entanglement density, segmental mobility, and relaxation dynamics [7]. For instance, long-chain branching increases melt elasticity and alters stress transfer across phases, while tacticity influences crystallization tendencies in semi-crystalline blends. These molecular features indirectly modulate miscibility by affecting the entropy of mixing and directly impact mechanical responses such as yield strength, toughness, and creep resistance.

In multi-component blends, thermodynamic compatibility between constituent polymers governs phase morphology. Depending on interaction parameters, compositions, and processing conditions, morphologies can range from homogeneous single-phase systems to phase-separated structures such as dispersed (sea–island), fibrillar, or co-continuous networks [8]. These morphologies exert a profound influence on bulk properties. For example, finely dispersed rubbery domains in a glassy matrix can enhance impact resistance through cavitation and shear banding, whereas co-continuous morphologies may optimize transport or damping properties. However, the mechanical benefits of immiscibility depend on interfacial tension, domain size distribution, and interfacial adhesion, which collectively determine stress-transfer efficiency and failure modes [9]. Consequently, predictive design requires simultaneous consideration of equilibrium thermodynamics and interfacial mechanics.

Recent theoretical developments underscore the importance of multi-scale modeling frameworks capable of bridging molecular descriptors with emergent macroscopic behavior [11]. Field-theoretic and self-consistent approaches have advanced understanding of phase-separation kinetics and equilibrium morphologies, refining the connections between Flory–Huggins interaction parameters and experimentally measurable quantities such as modulus, toughness, and viscoelastic spectra [12]. Despite these advances, classical theories often assume monodispersity and near-equilibrium conditions, limiting their applicability to real-world polymer blends that exhibit polydispersity, chain entanglement heterogeneity, and processing-induced non-equilibrium states [13].

As a result, recent literature increasingly emphasizes the need for integrative frameworks that fuse molecular-level descriptors (e.g., chemical functionality, chain topology) with mesoscopic morphology and macroscopic performance metrics. Such approaches aim to generate predictive property maps, enabling visualization of trade-offs between stiffness, toughness, processability, and sustainability across compositional and structural design spaces [18]. These challenges motivate the incorporation of data-driven tools to complement and extend traditional theory.

Machine learning applications in polymers and soft matter

Machine learning (ML) has rapidly emerged as a powerful methodology for addressing the intrinsic complexity of polymer and soft matter systems, where non-linear interactions and high-dimensional parameter spaces hinder purely physics-based prediction [10]. In polymer blend research, supervised learning algorithms, including random forests and kernel-based methods, have been employed to map composition–structure–property relationships, enabling accelerated screening of candidate formulations without exhaustive experimentation or simulation [14]. These models are particularly effective at capturing non-linear responses arising from coupled effects of composition, molecular weight, and processing conditions.

Unsupervised learning techniques, such as clustering and dimensionality reduction, have been applied to large datasets of phase behavior and morphology descriptors, revealing latent organizational patterns that are not evident through conventional analysis [15]. Such methods aid in identifying morphological similarity regimes and transition boundaries, thereby enhancing the interpretability of complex blend landscapes. Furthermore, several studies demonstrate ML's

capacity to act as a surrogate for computationally expensive simulations, achieving high-fidelity predictions of properties such as solubility parameters, glass transition temperatures, and viscoelastic moduli [19, 21].

Beyond forward prediction, ML has enabled inverse design paradigms in soft matter systems, wherein target properties—such as toughness, permeability, or recyclability—serve as inputs to identify optimal structural or compositional configurations [22]. For polymers, graph-based and neural network representations have proven especially promising, as they encode chain connectivity and topology more naturally than traditional descriptor sets, uncovering structure–property correlations overlooked by linear or low-dimensional regression models [23].

Nevertheless, persistent challenges limit widespread deployment. Polymer datasets remain relatively scarce and heterogeneous, and developing robust polymer representations capable of encoding sequence, conformation, and intermolecular interactions remains an open problem [24]. Studies increasingly converge on hybrid modeling strategies that integrate physics-based priors—such as thermodynamic constraints or scaling laws—into data-driven architectures, improving generalization, interpretability, and extrapolative capability [26, 28]. This convergence signals a broader methodological shift toward unified frameworks that balance physical insight with statistical learning, aligning closely with emerging goals for sustainable, trade-off-aware polymer design.

Explainable AI techniques and their relevance to materials science

Explainable Artificial Intelligence (XAI) has emerged as a response to the interpretability deficit inherent in many high-performing machine learning (ML) models, particularly deep and ensemble-based approaches [16]. While such models excel at capturing non-linear, high-dimensional relationships, their opacity limits scientific insight and hampers adoption in knowledge-driven fields such as materials science. XAI addresses this limitation by introducing either post-hoc interpretability methods, which analyze trained models after prediction, or intrinsically interpretable architectures, which embed transparency into the model structure itself.

Among post-hoc approaches, SHapley Additive ExPlanations (SHAP) have gained prominence due to their firm grounding in cooperative game theory and their ability to provide consistent, additive feature attributions [17]. In materials datasets, SHAP values can decompose predictions into contributions from molecular descriptors, compositional variables, or processing parameters, thereby illuminating how specific structural elements influence predicted properties. Complementarily, Local Interpretable Model-Agnostic Explanations (LIME) approximate complex models with simpler surrogate models in the vicinity of a given prediction, enabling localized interpretability even in highly non-linear, high-dimensional spaces [20]. Such a locality is particularly valuable in materials design, where property trends may differ across narrow regions of composition or morphology.

In materials science, XAI plays a critical role in aligning ML outputs with established physical intuition, thereby enhancing model trustworthiness and scientific utility [25]. For example, feature importance analyses have successfully identified key descriptors governing electronic band gaps in semiconductors, providing mechanistic insights consistent with quantum and solid-state theories [27]. These successes offer a compelling analogy for polymer and soft matter systems, where disentangling the contributions of molecular architecture, phase morphology, and interfacial effects remains a central challenge.

Emerging applications of XAI in soft matter physics further demonstrate its potential. In rheological modeling, attribution methods have been used to interpret ML-predicted viscoelastic responses, revealing how flow conditions induce microstructural rearrangements and transitions between deformation regimes [29]. Such insights bridge phenomenological observations with underlying structural dynamics, highlighting XAI's capacity to function as a hypothesis-generating tool rather than merely an explanatory add-on. Nonetheless, most existing XAI implementations assume relatively homogeneous or unimodal data representations, limiting their applicability to complex systems such as polymer blends that exhibit simultaneous variation in chemistry, morphology, and processing history [30].

Integration of XAI in structure–property mapping for polymer blends

Synthesizing these developments, XAI offers a promising pathway toward interpretable structure–property maps for polymer blend systems, where competing mechanisms and trade-offs obscure direct causal relationships [1, 2]. Recent studies have begun applying attribution-based methods to ML-predicted phase diagrams, identifying dominant variables —such as chain length, interaction parameters, or composition asymmetry—that govern phase stability and transition boundaries [3, 4]. These efforts demonstrate the feasibility of extracting physically meaningful trends from data-driven models, even when trained on sparse or heterogeneous datasets.

However, significant gaps remain. Current approaches rarely span multiple length scales, and few explicitly incorporate uncertainty quantification, which is essential for assessing confidence in predictions derived from limited experimental data or extrapolation into unexplored regimes [5, 31]. Moreover, polymer blends often generate multi-modal data—combining molecular descriptors, morphological images, and rheological time series—posing challenges for conventional XAI techniques that operate on fixed-length feature vectors. These challenges motivate a conceptual visualization of how explainable models can jointly represent predicted properties, attribution patterns, and uncertainty in polymer blend systems, as shown in **Figure 1**.

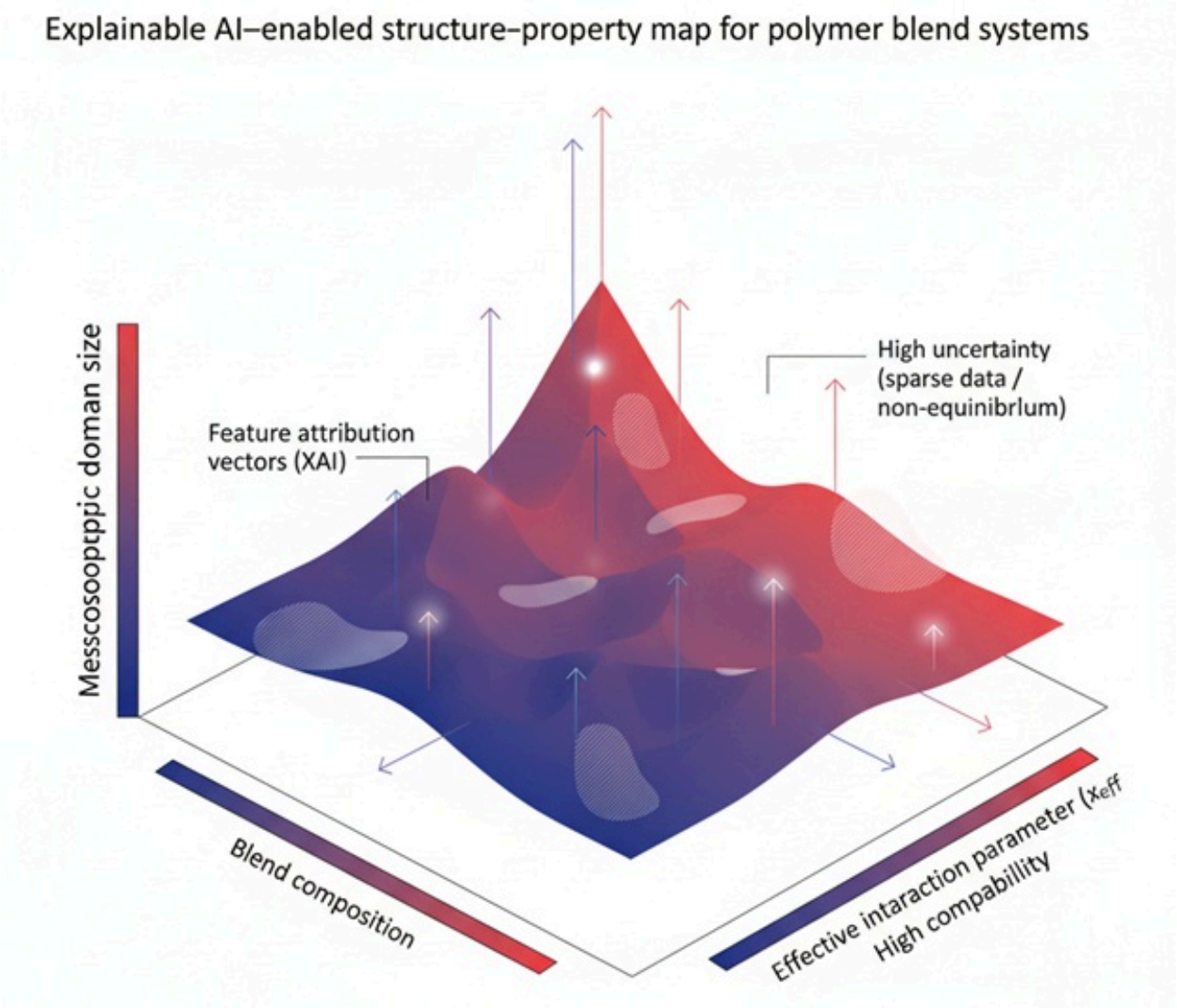

Figure 1. Conceptual explainable AI–enabled structure–property landscape for polymer blends, showing predicted property, local feature attributions, and high-uncertainty regions

The literature increasingly emphasizes the transformative potential of XAI in reshaping theoretical inquiry within materials science [32, 33]. By revealing latent structure–property correlations and highlighting unexpected drivers of performance, XAI-enabled models can stimulate new hypotheses, guide targeted experiments, and refine existing physical theories. This perspective reframes XAI not as a compromise between accuracy and transparency, but as a conceptual bridge that integrates data-driven prediction with mechanistic understanding. To make explicit how interpretability can operate across structural scales in polymer blends, the relationships between representative descriptors, target properties, and explanatory roles are organized in **Table 1**.

Table 1. Multi-scale descriptors, predicted properties, and XAI interpretability roles in polymer blend systems

Structural scale	Representative descriptors	Target properties	ML role	XAI contribution	Theoretical insight enabled
Molecular	Chain length, polarity, tacticity, and branching	Tg, modulus	Non-linear feature learning	Feature attribution (SHAP)	Entropic vs enthalpic dominance
Mesoscopic	Domain size, phase continuity, interfacial area	Toughness, permeability	Morphology–property mapping	Causal mediation analysis	Phase-mediated property emergence
Macroscopic	Blend ratio, processing conditions	Impact strength, recyclability	Global property prediction	Counterfactual explanations	Trade-off sensitivity and stability
Cross-scale	Hierarchical descriptors	Multi-objective performance	Ensemble learning	Uncertainty-aware explanations	Robust design boundaries

Overall, the synthesis of recent work suggests clear opportunities for novel conceptual frameworks in polymer blend research—frameworks that prioritize interpretability, scalability, and awareness of uncertainty without sacrificing predictive power [34, 35]. Such developments align naturally with broader goals of trade-off-sensitive and sustainable materials design, positioning XAI as a foundational component of next-generation structure–property modeling.

Proposed conceptual framework

The proposed conceptual framework, termed the interpretable structure–property mapping framework (ISPMF) for polymer blend systems, is a novel theoretical construct designed to harness explainable AI to generate transparent and actionable structure–property maps. Unlike existing models that treat AI as opaque predictors, ISPMF conceptualizes a modular architecture in which interpretability is embedded at each stage, drawing on soft-matter principles to ensure alignment with thermodynamic realities [1, 6]. The conceptual departure of the proposed framework from traditional and black-box approaches—particularly with respect to interpretability, uncertainty awareness, and multi-scale reasoning—is clarified through the comparison presented in **Table 2**.

Table 2. Comparison of traditional, AI-driven, and XAI-enabled structure–property mapping frameworks

Aspect	Traditional models	Black-box ML	Existing XAI in materials	ISPMF (This work)

Interpretability	High, but limited	Low	Moderate, post-hoc	High, recursive, and embedded
Multi-scale integration	Partial	Implicit	Limited	Explicit, hierarchical
Uncertainty awareness	Rare	Often absent	Occasionally included	Core design principle
Theoretical insight	Strong but narrow	Weak	Emerging	Central objective
Applicability to blends	Phenomenological	Data-dependent	Nascent	Tailored explicitly

At its foundation, ISPMF posits a tripartite structure: an input module for multi-scale descriptors, a core processing module integrating AI with XAI interpreters, and an output module for visualized maps with embedded explanations. The input module aggregates descriptors across scales—molecular (e.g., monomer polarity), mesoscopic (e.g., domain size distributions), and macroscopic (e.g., blend ratio)—framed as a unified feature space informed by recent literature on polymer representations [10, 11]. This avoids reductionism by preserving hierarchical relationships, a departure from flat-feature approaches in prior works [14].

The core module employs ensemble AI models, such as adaptive boosting, to predict properties while quantifying uncertainties, enhancing robustness in blend scenarios prone to variability [16, 17]. Crucially, XAI layers—incorporating SHAP for global attributions and counterfactuals for local what-if analyses—decompose predictions into causal contributions. For instance, in a hypothetical immiscible blend, ISPMF might attribute enhanced elasticity to interfacial reinforcement, providing theoretical insights absent in black-box mappings [20, 21].

The output module manifests as interpretable maps, conceptualized as multi-dimensional landscapes where contours represent property gradients, overlaid with explanation vectors indicating feature influences [25, 26]. This fosters a dialogic interaction between theory and prediction, enabling refinements in conceptual models of phase behavior [28, 29].

In essence, ISPMF advances originality by framing interpretability as a recursive process in which explanations feed back to refine inputs, contrasting static frameworks in the literature [32, 33]. This promotes a theoretical shift toward AI as a tool for discovery in soft matter. The flow of information from hierarchical microstructural descriptors through explanation-aware learning to interpretable property landscapes within the proposed framework is conceptually synthesized in **Figure 2**.

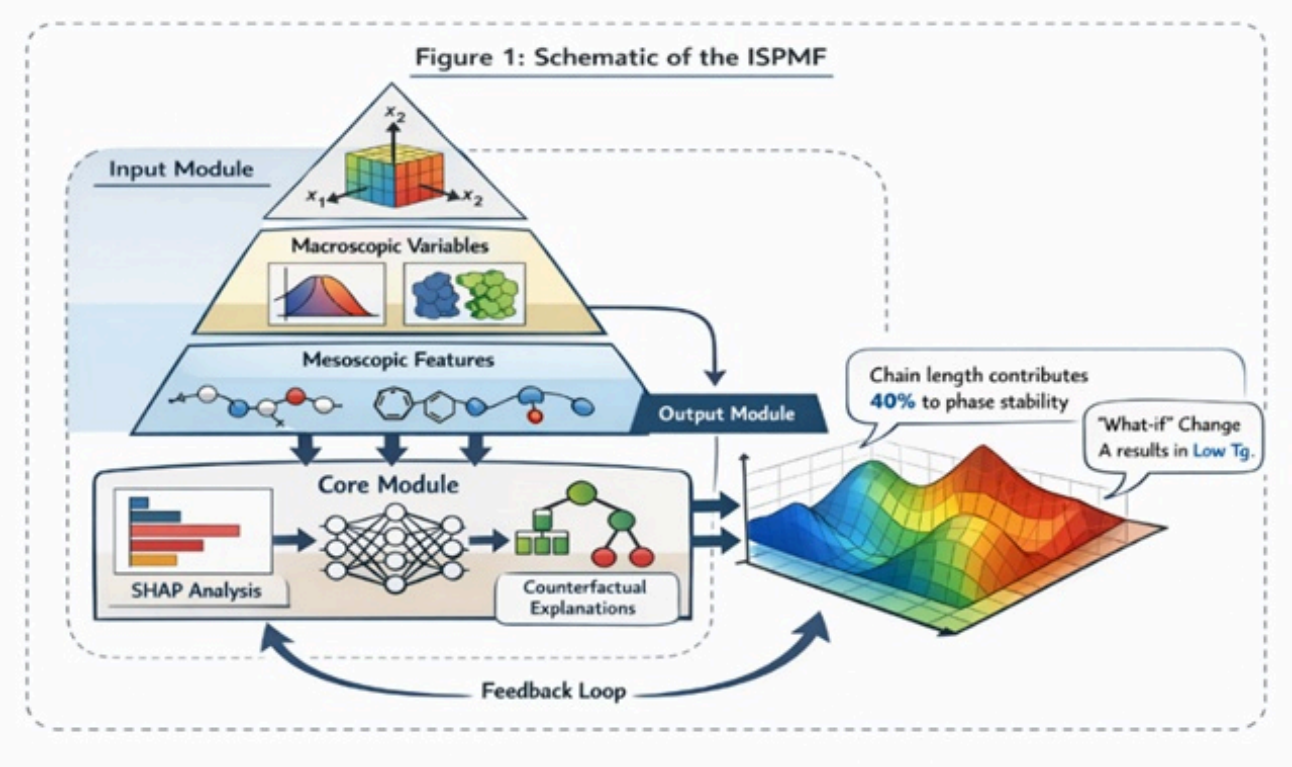

Figure 2. Schematic overview of the integrated structure–property modeling framework (ISPMF). Inputs organized as a hierarchical pyramid flow into a neural network core with embedded XAI tools, generating a color-coded 3D property map that highlights model predictions and explanatory insights. Feedback loops denote iterative learning within defined conceptual boundaries

Theoretical commitments and interpretive implications of the ISPMF

The interpretable structure–property mapping framework (ISPMF) embodies a set of explicit theoretical commitments for meaningfully integrating explainable AI into the study of polymer blend systems. Rather than articulating propositions or hypotheses, this section clarifies the interpretive logic, epistemic assumptions, and conceptual implications that follow directly from the framework's structure. These commitments define how structure–property reasoning is constrained, mediated, and rendered interpretable within ISPMF, without presupposing empirical validation.

Multi-Scale mediation as a condition for meaningful structure–property reasoning

A foundational commitment of ISPMF is that structure–property relationships in polymer blends cannot be meaningfully interpreted without explicit mediation across structural scales. Molecular descriptors, such as chain length or polarity, do not directly affect macroscopic properties; instead, their influence is mediated by mesoscopic phase morphologies and interfacial architectures [1, 3]. ISPMF therefore treats mesoscopic structure as an epistemically privileged layer, enabling interpretable maps that expose how phase continuity, domain size, and interfacial area condition macroscopic performance beyond direct molecular–property correlations.

Uncertainty awareness as an epistemic boundary

ISPMF explicitly incorporates uncertainty not as a numerical accessory, but as a conceptual boundary that delineates regions where structure–property inference is warranted from those where interpretation must remain provisional [5, 8]. In polymer blends, such uncertainty often arises from kinetic trapping, incomplete phase separation, or sparse data coverage. By embedding uncertainty into interpretable maps, the framework enables the identification of under-explored

or unstable compositional regimes, reinforcing epistemic restraint rather than forced inference in regions dominated by non-equilibrium effects.

Counterfactual reasoning as a conceptual design instrument

The framework commits to counterfactual explanation as a legitimate theoretical tool for exploring hypothetical structure–property relationships without empirical execution. Within ISPMF, counterfactuals enable systematic reasoning about how marginal structural changes—such as altered interfacial compatibility or domain connectivity—would conceptually influence emergent properties, such as permeability or toughness [10, 12]. This shifts counterfactual analysis from optimization rhetoric to structured conceptual exploration, supporting theory development in soft matter systems where direct experimentation may be infeasible.

Recursive interpretability and self-refinement

ISPMF advances the idea that interpretability is not static but recursive. Feature attributions and explanatory patterns generated by XAI are not treated as final interpretations, but as inputs for refining descriptor selection, scale coupling, and domain constraints [14, 16]. This recursive logic conceptualizes interpretability as a self-correcting process, enabling progressive clarification of structure–property reasoning as domain knowledge is iteratively incorporated.

Collective interpretability and bias mitigation

The modular architecture of ISPMF supports aggregating multiple interpretive lenses, reducing dependence on any single attribution mechanism. By conceptually allowing ensemble interpretability—where multiple XAI perspectives are reconciled—the framework mitigates bias arising from polymorphic phase behavior or descriptor dominance in polymer blends [21, 22]. This commitment strengthens causal plausibility in structure–property maps, particularly in systems exhibiting competing morphologies or non-monotonic property responses.

Trade-Off sensitivity and non-monotonic landscapes

ISPMF treats non-monotonic property trends not as anomalies, but as expected features of polymer blend landscapes. Interpretable maps generated within the framework are structured to reveal optima, plateaus, and trade-offs—such as stiffness–toughness or permeability–stability relationships—arising from intermediate miscibility or competing entropic and enthalpic contributions [25, 26]. This enables theory-guided exploration of design compromises without presuming linear or monotonic behavior.

Cross-System generalization through structural motifs

A further implication of ISPMF is that interpretable maps can support comparative reasoning across chemically distinct polymer systems by highlighting recurring structural motifs associated with similar property pathways [30, 31]. This enables a form of conceptual generalization in soft matter theory, where interpretability supports abstraction beyond individual chemistries toward transferable structural principles.

Physics-informed filtering of representation space

Finally, ISPMF commits to integrating domain-knowledge priors as epistemic filters rather than as performance enhancers. Physics-informed constraints—such as thermodynamic consistency or entropic dominance—serve to suppress spurious correlations and clarify interpretive signals in structure–property maps [33, 34]. This reinforces the role of explainable AI as a partner to soft matter theory rather than a substitute for it.

Collectively, these commitments define ISPMF as a framework for interpretable reasoning rather than predictive assertion. They position explainable AI as a conceptual instrument for interrogating structure–property relationships in polymer blends, supporting theory development while maintaining epistemic discipline [18, 20, 35].

Results and Discussion

The ISPMF represents a conceptual leap in applying XAI to polymer blends, addressing the opacity that hampers AI's integration into theoretical materials science. By prioritizing interpretability, the framework aligns data-driven predictions with foundational principles of soft matter, such as entropy-driven mixing and enthalpic interactions [2, 4]. This synergy mitigates the risk of spurious correlations, a common pitfall in ML applications to high-dimensional systems [6, 7].

One key implication is the facilitation of rational design in sustainable polymer blends. For instance, interpretable maps could theoretically guide the incorporation of bio-derived components, elucidating how structural compatibility influences recyclability without relying on trial-based approaches [9, 11]. This extends to industrial contexts, where transparency in property predictions could streamline formulation processes, reducing resource expenditure [13, 15].

However, conceptual challenges persist. The framework assumes comprehensive descriptor sets, yet soft matter's inherent stochasticity—arising from conformational variability—may introduce irreducible uncertainties [17, 19]. Moreover, while XAI techniques like SHAP provide attributions, their fidelity in capturing non-linear, multi-scale interactions requires theoretical scrutiny [21, 22]. Future extensions could incorporate graph-based representations to model network-like blend morphologies, enhancing causal inference [23, 24].

Ethically, ISPMF promotes accountable AI by demystifying decision-making, a crucial step in materials science, where predictions inform safety-critical applications [25, 26]. In contrast to generic XAI frameworks, ISPMF's tailoring to polymers ensures relevance to domain-specific queries, such as compatibilizer effects on phase stability [27, 28].

Limitations include the conceptual reliance on ensemble models, which, while robust, may obscure granular insights if not paired with intrinsic interpretability methods [29, 30]. Nonetheless, ISPMF's modularity allows for theoretical adaptations, potentially integrating quantum-derived descriptors for atomic-scale precision [31, 32]. Overall, this framework catalyzes a discourse on AI as an interpretive lens, enriching theoretical narratives in soft matter [33, 34].

Conclusion

This manuscript has developed the interpretable structure–property mapping framework (ISPMF) as a novel conceptual contribution to the integration of explainable artificial intelligence in polymer blend systems. Rather than advancing an algorithmic pipeline or empirical model, the work articulates a framework-level perspective on how structure–property maps can be rendered interpretable, uncertainty-aware, and theoretically meaningful within the context of soft matter materials science.

By synthesizing recent literature across polymer physics, machine learning, and explainable AI, the framework clarifies how multi-scale descriptors, interpretive mechanisms, and uncertainty representations can be coherently combined to support causal reasoning in complex blend systems. ISPMF reframes structure–property mapping as an epistemic process in which explanations, rather than predictions alone, serve as the primary carriers of scientific insight.

Crucially, the contribution of ISPMF lies in its explicit theoretical commitments: to scale mediation, interpretability as a recursive process, uncertainty as a boundary of inference, and domain knowledge as a constraint on meaning. These commitments position explainable AI not as a post-hoc transparency tool, but as a foundational element in the construction of structure–property understanding for polymer blends.

In doing so, this work advances a broader paradigm for applied artificial intelligence in materials science—one in which AI augments theoretical inquiry, supports trade-off-sensitive and sustainable materials design, and respects the epistemic limits inherent to complex soft matter systems. ISPMF thus provides a durable conceptual foundation for future advances in interpretable, physically grounded AI-assisted materials reasoning.

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