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Boundary Conditions of Transfer Learning in Materials Science: A Conceptual Theory of When Knowledge Transfers Fail

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Abstract

Transfer learning has emerged as a pivotal strategy in materials science, enabling the reuse of knowledge from data-rich domains to inform predictions in data-scarce contexts, thereby accelerating discovery across alloy design, nanomaterials, and functional compounds. Despite its growing adoption, the effectiveness of transfer learning remains contingent on subtle boundary conditions that delineate productive knowledge integration from ineffective or counterproductive transfer. This conceptual paper develops a theoretical framework to interpret these boundaries by examining interaction dynamics between source and target domains in materials contexts. It explores how mismatches in representational hierarchies—such as between atomic-scale and macroscopic descriptions—disrupt knowledge flow and yield distorted predictive outcomes. Systems-level analysis reveals trade-offs in model adaptability, where reliance on pre-trained representations may obscure emergent properties specific to target materials. Ethical considerations further highlight the risks of bias propagation from simulated to experimental domains, with implications for research prioritization and resource allocation. By integrating perspectives from materials informatics and complexity theory, the framework articulates steering logics to mitigate transfer failures through adaptive feature alignment. This work advances conceptual understanding of transfer learning limitations and provides interpretive guidance for future AI integration in materials science, without empirical validation.

Keywords Materials informatics, Feedback dynamics, Transfer learning, Knowledge boundaries, Domain interactions, Epistemic uncertainties

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Introduction

AI-Driven transformation in materials science

The integration of artificial intelligence (AI) into materials science has fundamentally reshaped traditional paradigms of materials discovery and design. Conventional trial-and-error methodologies—often time-consuming and resource-intensive—are increasingly being replaced by data-driven frameworks that exploit large-scale computational power. Among these advances, transfer learning has emerged as a particularly influential technique, enabling the reuse of knowledge acquired in one domain to enhance predictive performance in another. This capability is especially valuable in materials science, where datasets frequently differ in size, quality, and representational fidelity. By leveraging knowledge from data-rich simulations to inform data-scarce experimental contexts, transfer learning facilitates the exploration of complex material phenomena, including phase transformations, mechanical responses, and electronic behaviors [1, 2].

However, despite its promise, transfer learning is constrained by intrinsic limitations that can hinder effective knowledge integration and, in some cases, lead to misleading or degraded predictions.

Conceptual foundations of transfer learning across material domains

At its core, transfer learning assumes that source and target tasks share underlying structural or physical commonalities. Pre-trained models can thus be adapted to new tasks with limited additional data, provided that these shared features remain relevant. In materials science, this assumption underpins applications such as transferring models trained on bulk crystalline systems to nanoscale materials or using quantum-mechanical simulations to inform macroscopic engineering predictions [3, 4]. Analytically, these transfers illuminate how knowledge propagates across domains: alignment in feature representations can yield significant efficiency gains, whereas misalignment can introduce systematic distortions. For example, in polymer composite systems, transferring insights from molecular dynamics simulations to predict viscoelastic behavior may fail if interfacial effects—critical at larger scales—are inadequately represented in the source domain, resulting in feedback mechanisms that amplify prediction uncertainty [5].

Multi-Scale systems and epistemic boundaries

Materials systems are inherently multi-scale, spanning atomic, mesoscopic, and continuum regimes, each governed by distinct physical principles. Transfer learning efforts that aim to bridge these scales must therefore address epistemic questions about the validity of domain-invariance assumptions. At this system's level, incomplete or inappropriate transfers risk embedding biases derived from idealized or oversimplified source models into real-world applications. Such biases raise ethical concerns, particularly when AI-driven predictions are used to guide sustainable materials development or critical engineering decisions [6, 7]. To address these challenges, steering strategies, such as selective fine-tuning of neural network layers, have been proposed to balance the retention of broadly applicable knowledge with the need for domain-specific adaptation.

Evidence of transfer failures and ontological mismatches

Recent literature increasingly acknowledges the presence of boundaries that constrain successful transfer learning in materials science. Empirical studies have documented failures when transferring models across fundamentally different material classes—for instance, from metals to ceramics—where variations in bonding mechanisms undermine the coherence of transferred representations [8, 9]. These failures suggest that limitations arise not solely from data scarcity but from deeper ontological mismatches in how material properties are encoded and learned. The interaction between computational and experimental domains further complicates this process, as noise and uncertainty in target datasets can propagate through adapted models, triggering cascading errors [10]. Collectively, these findings highlight the need to conceptualize transfer learning limitations as boundary conditions rather than isolated technical shortcomings. The principal boundary conditions that govern when transfer learning shifts from facilitative to obstructive behavior across materials domains are summarized in **Table 1**.

Table 1. Boundary conditions governing successful and failed transfer learning in materials science

Boundary dimension	Source–target relationship	Mechanism of failure	Analytical interpretation	Systems-level consequence
Scale compatibility	Atomic → mesoscale/bulk	Loss of emergent phenomena (e.g., interfaces, defects)	Feature representations encode scale-specific invariants that do not generalize	Apparent accuracy masks degraded physical relevance
Physical regime alignment	Classical → quantum/multi-	Ontological mismatch in	Learned correlations violate target-domain	Cascading prediction instability under regime

	physics	governing laws	physics	shifts
Material class similarity	Metals → ceramics/polymers	Bonding and deformation mechanisms diverge	Latent spaces conflate incompatible property drivers	Negative transfer and reduced extrapolative robustness
Data fidelity gradient	Simulated → experimental	Noise asymmetry and idealization bias	Source features overfit smooth distributions	Brittle adaptation to real-world variability
Representation hierarchy	Local descriptors → global behavior	Missing long-range interactions	Feature abstraction collapses causal structure	Systematic underestimation of uncertainty
Contextual transfer assumptions	Generic → application-specific	Implicit invariance assumptions persist	Domain specificity is overwritten during fine-tuning	Overconfident decision support outputs

Analytical and systems-level implications

From an analytical perspective, transfer learning failures prompt a reassessment of how robustness is defined and evaluated within materials informatics. Trade-offs between computational efficiency and predictive fidelity become increasingly evident when transferred models encounter domain boundaries. This has motivated interest in hybrid modeling strategies that explicitly incorporate domain knowledge to stabilize cross-domain interactions [11]. Systems-level analyses further reveal feedback structures in which early transfer successes may obscure latent instabilities, which only become apparent under changing environmental conditions, such as temperature or pressure variations [12]. Epistemic reasoning plays a critical role here, particularly in interrogating assumptions of feature invariance that may not hold for polymorphic or highly heterogeneous materials [13].

Toward a boundary-centered conceptual framework

Building on these insights, this work advances a conceptual framework that interprets transfer learning failures through the lenses of complexity, adaptability, and boundary conditions. In semiconductor research, for example, transfers from density functional theory (DFT)-based models to device-level predictions often encounter quantum-to-classical transitions that disrupt learned representations; targeted adjustments in feature engineering can partially mitigate these effects [14]. Ethical considerations further underscore the importance of transparent reporting of transfer assumptions, helping to prevent overconfidence in AI-assisted materials decisions and supporting responsible innovation [15].

Contribution and scope of this study

Ultimately, this study reframes transfer learning failures not as isolated anomalies but as manifestations of broader systemic interactions inherent to materials science. By explicitly delineating the boundary conditions that govern when knowledge transfer shifts from facilitative to obstructive, the proposed framework contributes to a more nuanced understanding of AI integration in materials research. This perspective aims to support the development of more resilient, interpretable, and ethically grounded transfer learning methodologies that respect the intrinsic complexity of material behaviors.

Theoretical Background and Literature Synthesis

Evolution of transfer learning in artificial intelligence

Transfer learning emerged within the broader field of machine learning as a response to the inefficiencies associated with training models from scratch on limited datasets. Conceptually, it draws on principles of knowledge reuse that parallel

human cognitive adaptation, wherein previously acquired knowledge informs new learning tasks [16]. Early formalizations of transfer learning were developed primarily in computer vision and natural language processing, domains characterized by large-scale, labeled datasets and hierarchical feature representations [17]. In these contexts, models are typically pre-trained on general-purpose datasets and subsequently fine-tuned for task-specific objectives, exploiting shared representational structures to enhance learning efficiency.

From an analytical standpoint, the success of transfer learning in core AI domains can be attributed to a relatively high degree of domain proximity between source and target tasks. Interaction dynamics in these settings are often well-behaved, as low-level features—such as image edges or syntactic patterns in text—remain transferable across applications. Systems-level insights thus frame early transfer learning as a strategy that optimizes computational efficiency while preserving predictive fidelity under conditions of representational alignment.

Migration of transfer learning to materials science

The migration of transfer learning into materials science gained momentum in the early 2020s, largely in response to the field's persistent data asymmetries. While computational materials science produces vast quantities of simulation data, experimental datasets remain comparatively scarce, expensive, and heterogeneous [18]. Transfer learning offered a conceptual bridge between these domains, enabling models trained on large-scale simulations to inform experimentally relevant predictions. This shift reframed materials discovery as an interconnected knowledge ecosystem rather than a collection of isolated computational studies.

Interaction dynamics during this migration reveal a transition from predominantly homogeneous transfers—within closely related tasks—to increasingly heterogeneous transfers, in which models trained on general AI applications or distinct materials classes are repurposed for specialized materials predictions [19]. Systems-level analyses highlight a critical trade-off: although transfer learning reduces computational costs and accelerates model deployment, it also introduces dependencies on the validity and fidelity of source data. In applications such as defect detection and microstructure characterization, inaccuracies embedded in the source domain may propagate into downstream predictions, amplifying uncertainty [20]. Analytically, these challenges stem from the fact that materials systems frequently violate the domain similarity assumptions that underpin successful transfer learning in traditional AI contexts, due to their inherent multi-physics and multi-scale nature [21].

Applications of transfer learning in materials informatics

Within materials informatics, transfer learning has been widely adopted to accelerate property prediction across diverse material classes, including organic molecules, polymers, and inorganic crystalline solids. A prominent application involves adapting models pre-trained on extensive density functional theory (DFT) databases to predict electronic properties, such as bandgaps, in emerging materials systems like perovskites [22]. Conceptual interpretations frame these applications as mechanisms for bridging epistemic gaps, wherein high-fidelity simulated knowledge informs empirical exploration, thereby enhancing the efficiency of high-throughput materials screening workflows [23].

Despite these successes, interaction dynamics expose significant vulnerabilities. In polymer science, for example, transferring knowledge from small-molecule datasets to macromolecular systems often results in scale mismatches that distort predictions of viscoelastic behavior [24]. Systems-level insights further reveal feedback structures in which localized improvements achieved through transfer learning may not generalize across broader compositional or structural spaces. This limitation is evident in alloy design, where models adapted for phase stability prediction can exhibit degraded performance under compositional perturbations or extrapolative regimes [25].

Ethical, analytical, and steering considerations

Beyond technical performance, ethical reasoning has become increasingly relevant in assessing transfer learning applications in materials science. Biased or incomplete source datasets may skew downstream predictions, potentially

influencing sustainability assessments or materials prioritization in unintended ways [26]. These concerns underscore the importance of transparency in documenting transfer assumptions and limitations.

In response to these challenges, steering logics have emerged as a means of stabilizing transfer processes. Hybrid strategies, such as multi-task learning frameworks, integrate auxiliary prediction tasks to constrain model adaptation and reduce overfitting to misaligned features [27]. Analytically, such approaches seek to balance efficiency gains with epistemic robustness, while systems-level perspectives emphasize their role in mitigating cascading errors across interconnected materials prediction pipelines.

Identified challenges in knowledge transfer within materials domains

Challenges in transfer learning for materials science center on domain divergences that disrupt knowledge coherence. Analytical implications point to negative transfer phenomena, in which source-target mismatches degrade performance, particularly in heterogeneous materials such as composites [28]. Interaction dynamics illustrate how feature irrelevance—e.g., atomic descriptors ineffective for mesoscale behaviors—can create feedback loops that amplify uncertainties [29].

Systems-level insights highlight data quality disparities; simulated sources often lack the noise and variability of experimental targets, resulting in brittle adaptations [30]. Epistemic reasoning questions the ontological alignment of domains, such as when quantum models fail to capture thermodynamic ensemble effects in target predictions [31]. Trade-offs emerge between computational and interpretive costs, where aggressive fine-tuning risks overwriting valuable source knowledge [32].

Further, ethical dimensions arise from the way failures disproportionately affect underrepresented material classes, potentially hindering equitable innovation [33]. Steering logics advocate for meta-learning approaches to detect and mitigate boundary crossings, fostering adaptive resilience [34].

Synthesis of literature on transfer failures and boundary conditions

Synthesizing recent literature, transfer failures in materials science manifest through interpretive lenses as breakdowns of domain-invariance assumptions. For example, transfers from bulk to nanoscale domains often fail due to emergent quantum confinement effects that are not accounted for in the sources. Conceptual interpretations frame these as boundary conditions—thresholds where knowledge integration shifts paradigms, from facilitative to obstructive [16].

Interaction dynamics reveal cascading effects; in catalytic materials, mismatches in surface representations lead to erroneous activity predictions, with feedback amplifying epistemic gaps [17]. Systems-level insights integrate these into broader trade-offs, where the pursuit of generality sacrifices specificity, as evidenced by failures in multi-fidelity modeling [18]. Ethical reasoning emphasizes the implications for research integrity, urging transparent boundary mapping to avoid misleading outcomes [19].

Overall, the synthesis underscores a need for frameworks that interpret failures holistically, guiding future applications toward robust, boundary-aware transfers.

Proposed conceptual framework

The proposed framework conceptualizes transfer learning failures in materials science as emergent from boundary conditions that govern knowledge integration across domains. At its core, it interprets these boundaries through interaction dynamics in which source and target domains intersect via feature spaces, model architectures, and contextual embeddings. Analytical implications suggest that failures arise not from isolated mismatches but from systemic feedback structures, in which initial domain alignments degrade as divergences escalate, for example, across scales (atomic to bulk) or across physics (classical to quantum).

Systems-level insights reveal trade-offs in adaptability: high source generality may enhance initial transfers but introduces epistemic distortions when target-specific emergent properties, like topological defects in 2D materials, are overlooked. Steering logics emphasize dynamic alignment, where iterative feature recalibrations mitigate boundary crossings, thereby fostering resilience in heterogeneous systems such as metal-organic frameworks. Ethical reasoning integrates considerations of bias propagation and advocates for interpretive transparency to ensure equitable knowledge flows.

Conceptually, the framework delineates three interlocking components: domain interfaces, transfer conduits, and failure amplifiers. Domain interfaces represent the ontological overlap, interpreted as shared representational motifs that facilitate initial knowledge migration. Transfer conduits embody the mechanistic pathways—e.g., parameter sharing or feature extraction—through which knowledge navigates boundaries, with dynamics modulated by data fidelity gradients. Failure amplifiers capture escalating interactions, such as noise-induced variances that feed back into model instabilities, particularly in multi-phase materials. **Table 2** systematizes the principal failure amplifiers identified in the framework and maps them to steering strategies that mitigate boundary-induced breakdowns.

Table 2. Transfer learning failure amplifiers and steering strategies across materials domains

Failure amplifier	Triggering boundary condition	Observed effect on transfer	Steering/mitigation logic	Epistemic benefit
Feature misalignment amplification	Scale or physics mismatch	Progressive distortion of predictions	Selective layer freezing and adaptive re-embedding	Preserves physically meaningful abstractions
Noise feedback escalation	Simulation–experiment disparity	Uncertainty compounds across iterations	Domain-aware regularization and noise modeling	Stabilizes learning under heterogeneous data
Representation collapse	Over-generalized pretraining	Loss of target-specific variability	Hybrid physics-informed constraints	Restores causal structure
Negative transfer lock-in	Ontological incompatibility	Performance degradation persists	Early boundary diagnostics and transfer abort criteria	Prevents misleading convergence
Bias propagation	Skewed source datasets	Systematic prioritization errors	Transparent boundary documentation and audits	Ethical accountability and interpretability
Adaptation overwrite	Aggressive fine-tuning	Source knowledge erosion	Multi-task or meta-learning control	Balances adaptability with retention

Epistemic insights highlight how these components interact to set boundary conditions, with thresholds in similarity metrics triggering shifts from convergent to divergent outcomes. For instance, in semiconductor heterostructures, transfers from silicon-based models to III-V compounds may amplify failures via bandgap misalignment dynamics.

As illustrated in **Figure 1**, the proposed framework conceptualizes knowledge transfer as a dynamic interaction between simulated and experimental domains, mediated by boundary conditions, feedback mechanisms, and adaptive steering logics.

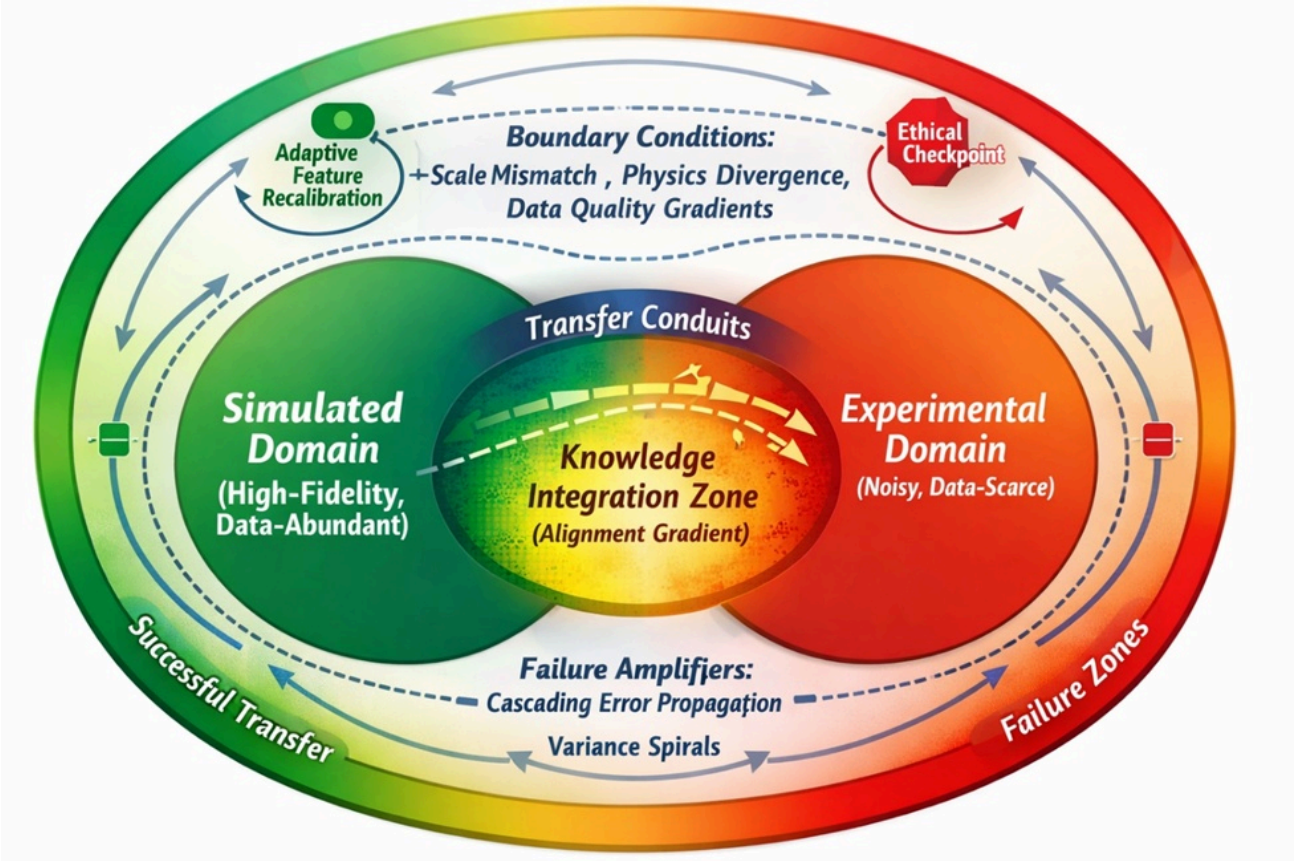

Figure 1. schematically depicts the multilevel interactions governing successful and failed knowledge transfer between simulated and experimental domains.

Conceptual and theoretical implications for transfer learning in materials science

The conceptual framework proposed in this study generates a set of theoretical implications that advance understanding of transfer learning dynamics in materials science. Central to these implications is the recognition that transfer learning is not a neutral process of knowledge reuse, but a boundary-sensitive mechanism in which the compatibility of representational assumptions determines epistemic validity. Boundary conditions—defined here as thresholds where domain correspondence weakens—play a decisive role in shaping how knowledge is integrated, transformed, or distorted during transfer.

At the level of interaction dynamics, misalignments between source and target domains emerge as primary drivers of epistemic instability. Structural incompatibilities, such as differences in lattice symmetry, bonding character, or dominant deformation mechanisms, can introduce recursive feedback effects that amplify uncertainty rather than attenuate it [1, 6]. In such cases, transferred representations may retain internal coherence while losing physical relevance, leading to plausible yet misleading interpretations of material behavior. This highlights a critical conceptual shift: transfer learning performance metrics alone are insufficient indicators of epistemic success, particularly when boundary conditions are crossed implicitly rather than explicitly acknowledged.

From a systems-level perspective, the framework underscores fundamental trade-offs between computational efficiency and representational fidelity. While transfer learning enables accelerated exploration of large material spaces by reducing training costs and data requirements, these gains may come at the expense of accurately capturing emergent properties. This tension is especially pronounced in nanostructured and low-dimensional systems, where quantum effects, surface phenomena, and size-dependent interactions diverge sharply from the classical approximations embedded in many

source models [10, 22]. Conceptually, this suggests that efficiency gains obtained through transfer learning must be contextualized within the physical regimes to which they are applied, rather than treated as universally beneficial.

The framework also extends into the ethical and normative dimensions of materials informatics. Failed or misaligned transfers can have downstream consequences beyond technical inaccuracies, particularly when AI-driven predictions inform decisions related to sustainable materials development, resource allocation, or environmental impact assessment. Biased source data or unexamined transfer assumptions may systematically skew research priorities, reinforcing existing inequities in materials selection or overlooking viable alternatives [15, 26]. Within this context, ethical reasoning becomes inseparable from conceptual model design, emphasizing the need for adaptive steering logics that actively monitor and realign feature spaces as domain conditions evolve.

Importantly, these conceptual implications resonate strongly with the growing adoption of multi-fidelity modeling strategies in materials science. Transfer learning is frequently positioned as a bridge between low-fidelity simulations and high-fidelity experimental data; however, the framework reveals that fidelity gradients themselves constitute boundary conditions that must be navigated deliberately. Without explicit recognition of these gradients, small discrepancies can be amplified through iterative model updates, producing cascading errors across scales [30, 32]. Iterative knowledge curation—where transferred representations are continuously evaluated against domain-specific constraints—emerges as a theoretically grounded strategy for mitigating such amplifier effects.

Collectively, these implications reposition transfer learning as an adaptive, boundary-governed epistemic process rather than a purely technical optimization tool. Conceptual rigor, domain awareness, and ethical accountability are thus framed as foundational requirements for sustainable and interpretable AI integration in materials science.

Results and Discussion

Integrating the framework's insights, the discussion centers on the broader interpretive ramifications for materials informatics. Feedback structures operating within boundary conditions suggest that transfer failures should be viewed as opportunities for epistemic refinement rather than as isolated technical shortcomings [2, 18]. Such failures expose latent assumptions about domain similarity and feature invariance, prompting deeper scrutiny of how knowledge representations evolve across material classes and scales.

The trade-off between model generalization and domain specificity invites a reassessment of hybrid modeling strategies. Interaction dynamics indicate that physics-informed constraints can play a stabilizing role in transfer learning, anchoring data-driven representations to established material principles and reducing susceptibility to misalignment-induced errors [8, 24]. These insights support a more integrative modeling philosophy in which AI systems are designed to complement, rather than replace, domain knowledge.

From a systems-level standpoint, collaborative paradigms that combine artificial intelligence with expert-driven interpretation are increasingly necessary to navigate the ethical challenges posed by bias propagation and uncertainty transfer [12, 28]. Steering logics such as modular feature selection and domain-aware adaptation emerge as particularly effective in complex material systems, including biomaterials, where biological interfaces introduce additional layers of variability and nonlinearity [4, 20]. These strategies reinforce the view that resilience in transfer learning arises from adaptive structure rather than algorithmic complexity alone.

Conclusion

This paper develops a boundary-centered conceptual theory for interpreting when and why transfer learning fails in materials science. Rather than treating negative transfer as an incidental technical outcome, the framework positions failure as an emergent consequence of boundary conditions—thresholds at which source–target compatibility breaks

across scales, physical regimes, data fidelity, representational hierarchies, and material classes. By foregrounding these boundaries, the study clarifies that transfer learning is an epistemic process as much as a computational one: models can preserve internal statistical coherence while losing physical relevance, producing predictions that appear plausible yet become misleading once boundary crossings occur.

The proposed framework integrates interaction dynamics and systems-level feedback to show how early apparent transfer success can obscure latent instabilities that later surface under perturbations, extrapolation, or regime shifts. The delineation of domain interfaces, transfer conduits, and failure amplifiers explains how mismatches are not merely additive but can self-reinforce through uncertainty escalation, representation collapse, and adaptation overwrite. In doing so, the work reframes robustness in materials informatics: evaluation must extend beyond aggregate error metrics toward boundary awareness, including explicit interrogation of invariance assumptions and fidelity gradients that mediate simulated-to-experimental transfer.

Beyond analytical implications, the theory strengthens the normative argument that boundary-blind transfer is not value-neutral. Bias propagation and overconfident generalization can distort research prioritization, sustainability assessments, and resource allocation, particularly for underrepresented material classes and noisy experimental regimes. Accordingly, the steering logics synthesized here—adaptive feature alignment, domain-aware regularization, early boundary diagnostics, and hybrid physics-anchored constraints—are not presented as mere performance enhancements but as mechanisms for epistemic accountability. In this sense, responsible transfer learning in materials science requires transparency about what is being transferred, under what assumptions, and where those assumptions fail.

Overall, this study contributes a conceptual foundation for designing boundary-aware transfer learning that respects the intrinsic multi-scale and multi-physics complexity of material behavior. By converting transfer limitations into interpretable boundary maps and actionable steering principles, the framework supports future AI integrations that are not only more efficient, but more reliable, interpretable, and ethically defensible—thereby advancing materials innovation without collapsing domain complexity into fragile generalization.

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