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From Property Prediction to Materials Narratives: A Conceptual Shift in Scientific Reporting

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Abstract

The evolution of materials science discourse reflects a transition from isolated property predictions toward integrated narratives that encapsulate multifaceted material behaviors and contexts. This conceptual manuscript explores the interpretive dynamics underlying this shift, emphasizing how narrative structures facilitate deeper epistemic integration across disparate data sources and theoretical lenses. By synthesizing recent advances in computational and artificial intelligence-driven approaches, the analysis highlights the interplay between predictive accuracy and narrative coherence, revealing trade-offs between representational fidelity and communicative efficacy. Conceptual interpretations underscore the role of narrative frameworks in bridging quantitative outputs with qualitative insights, fostering systems-level understandings that accommodate uncertainty and contextual variability. Ethical considerations arise in balancing narrative persuasion with scientific rigor, while epistemic reasoning examines how such shifts influence knowledge dissemination in interdisciplinary settings. The proposed framework delineates steering logics that guide the transformation of predictive models into narrative constructs, and illustrates feedback structures that enhance interpretability without making empirical assertions. This shift invites reflection on the broader implications for scientific reporting, where narratives serve as interpretive scaffolds for complex material phenomena, promoting holistic engagement over fragmented prognostications. Ultimately, the manuscript advocates for a nuanced appreciation of narrative's integrative potential in reshaping materials discourse.

Keywords Materials narratives, Property prediction, Conceptual shift, Scientific reporting, Epistemic integration, Narrative coherence

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Introduction

The discourse within materials science has long been anchored in the pursuit of precise property predictions, where computational models and empirical validations serve as cornerstones for understanding material behaviors under varied conditions. This paradigm, rooted in quantitative assessments, has enabled significant advancements in fields such as alloy design, polymer engineering, and nanomaterial applications by focusing on discrete, measurable metrics, such as tensile strength, thermal conductivity, and the electronic bandgap. This approach has built a robust edifice of knowledge, transforming materials science into a highly predictive discipline capable of guiding the synthesis of novel substances with tailored functions.

However, as the complexity of materials systems escalates—encompassing multiscale interactions, environmental dependencies, and lifecycle considerations—a conceptual reevaluation emerges, one that critically pivots toward narrative forms of scientific reporting. This shift does not negate the foundational value of quantitative predictions but

rather seeks to reinterpret them within broader, interconnected stories that reveal underlying dynamics and contextual interplays [1, 2]. Where a predictive model might output a singular value for corrosion resistance under specific conditions, a narrative framework would contextualize that value within a story of the material's journey: its synthesis pathway, the evolution of its grain boundaries in service, its interaction with fluctuating environmental agents, and its eventual failure modes. This narrative captures the why and how behind the what, exposing the relational logic that pure quantification often obscures.

At its core, this transition involves a fundamental reconceptualization of how materials knowledge is structured, validated, and conveyed. Traditional property prediction emphasizes isolating variables and optimizing for deterministic outcomes, often distilled into authoritative numerical values or graphical representations. In contrast, materials narratives weave these discrete data points into cohesive, causal accounts. For example, a narrative might integrate data on a catalyst's surface energy, its nanoparticle size distribution, and its temporal activity decay to tell a story of sintering and poisoning under reaction conditions. This story explains performance trends more powerfully than any single plot of conversion versus time [3, 4].

Such narratives foster critical interpretive depth, allowing stakeholders—from researchers and engineers to policymakers and end-users—to engage with materials science in a more holistic, strategic manner. They transform data into insight by highlighting relational aspects: how a polymer's entanglement density (a microstructural narrative) dictates not only its melt viscosity but also its processability in additive manufacturing and its ultimate toughness in a final product. This interpretive lens underscores the inherent limitations of purely predictive, siloed approaches, which risk overlooking emergent phenomena, path dependencies, or systemic feedback loops that defy straightforward quantification. The narrative turn thus represents not an abandonment of precision but an embrace of complexity, positioning each prediction as a pivotal event within a richer, more accountable story of material behavior and its societal implications.

This conceptual exploration draws from the integration of artificial intelligence (AI) and large language models (LLMs) in materials research, which has expanded the toolkit for data synthesis and interpretation. AI-driven tools facilitate the aggregation of vast datasets, but their true interpretive power lies in generating narrative overlays that contextualize predictions within theoretical frameworks and practical scenarios [5, 6]. For instance, the interplay between machine learning outputs and human-readable explanations reveals trade-offs between accuracy and comprehensibility, and narratives act as mediators to resolve these tensions. Epistemic reasoning further illuminates how this shift enhances knowledge accessibility, particularly in interdisciplinary collaborations where domain-specific jargon might otherwise impede understanding [7, 8].

Ethically, the move toward narratives introduces considerations of representational equity, ensuring that diverse perspectives—such as those from sustainability or societal impact assessments—are incorporated without bias. Feedback structures inherent in narrative construction allow for iterative refinement, in which initial predictive insights are revisited through contextual lenses, promoting a dynamic rather than static view of the materials [9, 10]. This interpretive approach aligns with broader trends in scientific communication, where the demand for transparency and reproducibility intersects with the need for engaging, story-driven expositions.

The manuscript's analytical focus centers on the conceptual implications of this shift, avoiding any empirical validations or methodological prescriptions. Instead, it synthesizes literature to uncover interaction dynamics between prediction-centric and narrative-oriented paradigms, highlighting how the latter enables systems-level insights into material complexities [11, 12]. By examining steering logics that guide narrative formation—such as the selection of thematic threads or the balancing of detail levels—the analysis reveals epistemic pathways for more inclusive scientific reporting. Trade-offs emerge between narrative flexibility and predictive precision: overemphasizing stories might dilute quantitative rigor, while underutilizing them could stifle innovative interpretations [13, 14].

In this context, the role of LLMs becomes particularly salient, not as predictors per se, but as facilitators of narrative synthesis. These models interpret vast corpora of materials literature, distilling patterns into coherent accounts that bridge

gaps between atomic-scale simulations and real-world applications [15, 16]. Conceptual interpretations here emphasize the ethical imperative to maintain narrative integrity, preventing the conflation of interpretive flair with unsubstantiated claims. Systems-level insights further demonstrate how narratives can encapsulate feedback loops, such as those between material design iterations and performance evaluations, fostering a recursive understanding of innovation cycles [6, 17]. **Table 1** contrasts prediction-centric and narrative-centric reporting paradigms, highlighting their distinct epistemic roles and complementary functions.

Table 1. Prediction-centric vs narrative-centric paradigms in materials science

Dimension	Property prediction paradigm	Materials narrative paradigm
Epistemic role	Establishes quantitative anchors and bounded expectations	Integrates predictions into relational, contextual meaning structures
Unit of knowledge	Isolated properties (e.g., strength, bandgap, conductivity)	Interconnected material trajectories across contexts and scales
Treatment of uncertainty	Residual to be minimized or bounded numerically	Interpreted as an intrinsic feature shaping narrative scope
Temporal framing	Largely static, snapshot-based	Explicitly temporal, incorporating lifecycle and evolution
Communicative mode	Numerical, graphical, model-centric	Relational, thematic, systems-oriented
Interpretive flexibility	Limited; constrained by model form	High; accommodates contextual variability
Risk profile	Overconfidence through apparent precision	Overreach through persuasive framing
Ethical exposure	Implicit, often backgrounded	Explicit, embedded through epistemic boundary marking
Primary strength	Precision and reproducibility	Coherence and integrative understanding
Primary limitation	Fragmentation of meaning	Dependence on disciplined steering logics

Ultimately, this introduction sets the stage for a deeper synthesis of theoretical backgrounds, leading toward a proposed framework that interprets the shift as an evolutionary step in scientific epistemology. By prioritizing conceptual interconnections over isolated assertions, the discourse invites reflection on how material narratives might redefine the boundaries of knowledge production and dissemination in an era of accelerating technological convergence [18, 19]. The ensuing sections will elaborate on these dynamics, ensuring a scholarly tone that privileges precision and integrative reasoning.

Theoretical Background and Literature Synthesis

Evolution of predictive paradigms in materials science: The foundational underpinnings of materials science have historically emphasized predictive paradigms, in which computational frameworks interpret atomic and molecular interactions to forecast macroscopic properties. This approach integrates quantum-mechanical principles with statistical mechanics, enabling the conceptualization of material behavior through layered abstractions [12, 20]. Interpretive dynamics within these paradigms reveal how predictive models serve as epistemic bridges, connecting theoretical constructs to observable phenomena without invoking empirical specifics. The synthesis of recent literature highlights a maturation in these models, in which interaction complexities—such as electron-phonon couplings or defect dynamics—are interpreted as systemic interdependencies rather than isolated variables [21, 22].

Trade-offs in representational accuracy emerge as a key theme, with steering logics balancing model simplicity and comprehensive coverage. For instance, the conceptual integration of machine learning architectures allows for the interpretation of high-dimensional data spaces, where predictive outputs are reframed as interpretive signals within broader material ecosystems [18, 19]. Ethical reasoning underscores the importance of epistemic humility in these interpretations, acknowledging inherent uncertainties that predictive frameworks cannot fully encapsulate. This subsection synthesizes how such paradigms have evolved, setting the conceptual groundwork for narrative expansions [12, 20].

Integration of AI and LLMs in interpretive frameworks: Artificial intelligence, particularly large language models, has introduced novel interpretive layers to materials discourse, facilitating the synthesis of disparate knowledge sources into unified conceptual structures. Literature from the past five years illustrates how LLMs function as interpretive agents, parsing textual and numerical data to uncover latent connections that enhance systems-level insights [1, 3]. The dynamics of this integration involve feedback loops, in which AI-generated interpretations iteratively refine human conceptualizations, promoting a symbiotic relationship between computational efficiency and narrative depth [5, 7].

Conceptual interpretations emphasize LLMs' role in navigating epistemic trade-offs, such as the tension between data-driven precision and contextual relevance. By synthesizing patterns from extensive literature corpora, these models enable the conceptualization of materials as narrative entities, where properties are not merely predicted but interwoven into stories of functionality and adaptation [9, 11]. Ethical considerations arise in ensuring that AI-assisted interpretations maintain scholarly integrity and avoid overreliance on algorithmic outputs that might obscure human oversight. This synthesis reveals how LLMs amplify interpretive capabilities, transforming raw predictions into multifaceted insights [13, 15].

Narrative structures in scientific communication: Narrative structures in scientific reporting offer an alternative lens for interpreting complex systems, shifting focus from discrete predictions to relational dynamics. Recent syntheses indicate that narratives serve as integrative tools, allowing for the conceptual weaving of predictive elements into coherent accounts that reflect material lifecycles and environmental interactions [2, 4]. Interaction dynamics within these structures highlight how narratives accommodate variability, providing epistemic flexibility where rigid predictions fall short [6, 8].

Systems-level insights derived from literature underscore the feedback mechanisms inherent in narrative construction, such as the recursive linkage between material properties and application contexts [10, 12]. Trade-offs in narrative adoption include the potential for interpretive richness versus communicative conciseness, with steering logics emphasizing selective emphasis on key themes. Ethical epistemic reasoning calls for transparency in narrative framing, ensuring that interpretations remain grounded in conceptual rigor [14, 16]. This subsection synthesizes how narratives enhance scientific discourse, bridging gaps left by traditional predictive approaches [17, 19].

Conceptual intersections and epistemic implications: The intersection of predictive and narrative paradigms yields profound epistemic implications, with the former's quantitative focus complementing the latter's qualitative depth. Literature synthesis demonstrates how these intersections foster hybrid interpretive frameworks, enabling a more nuanced understanding of material complexities [6, 18]. Dynamics of interaction at these junctures involve balancing predictive certainty with narrative ambiguity, highlighting trade-offs in knowledge representation [12, 21].

Systems-level insights emphasize the role of feedback structures in sustaining epistemic coherence, as narratives reinterpret predictive outputs through contextual lenses [12, 18]. Ethical considerations in this synthesis stress the need for inclusive interpretations that account for interdisciplinary perspectives, preventing conceptual silos [20, 22]. Steering logics guide the navigation of these intersections, promoting integrative reasoning that enriches scientific reporting without diluting core principles [19, 20]. Overall, this background synthesis illuminates the conceptual pathways toward a narrative-centric shift, preparing the ground for the development of a framework [18, 21-23].

Proposed conceptual framework

The proposed framework conceptualizes the transition from isolated property prediction toward materials narratives as a structured epistemic transformation rather than a rhetorical embellishment. Instead of treating predictive outputs as terminal scientific claims, the framework repositions them as interpretive nuclei embedded within broader narrative architectures that enable systems-level sense-making.

At its core, the framework distinguishes between quantitative anchors—formal predictions, confidence intervals, and learned correlations—and qualitative expansions that contextualize these anchors within material histories, usage conditions, societal constraints, and value-laden considerations. Narratives, in this sense, are not substitutes for prediction but epistemic envelopes that scaffold meaning, coherence, and interpretive continuity across scales.

Central to the framework are steering logics that regulate how predictive cores evolve into narrative structures. These logics operate through recursive feedback: initial predictions seed narrative development, narratives reshape interpretive priors, and revised priors recalibrate how subsequent predictions are understood. This recursive coupling mitigates the classical trade-off between precision and comprehensiveness by allowing narrow predictive accuracy to coexist with broader explanatory coherence—without inflating empirical claims.

Ethical reasoning is embedded as a boundary condition, not an external add-on. The framework emphasizes epistemic balance, ensuring that narratives amplify interpretability while preserving the integrity and limitations of predictive evidence. Rather than encouraging speculative overreach, narrative structures function as constraint-aware sense-making devices that explicitly mark uncertainty, scope, and contextual dependence.

From a systems perspective, the framework accommodates multilayered interactions: intrinsic material attributes (e.g., microstructure, thermodynamic tendencies) are interwoven with extrinsic dimensions (e.g., environmental exposure, application contexts, sustainability horizons). This layered coupling fosters a recursive understanding of material adaptability, where meaning evolves through interaction rather than static classification.

The framework is structured around three interdependent components:

1. Predictive Nuclei

Compact, quantitative cores representing aggregated model outputs and uncertainty-aware property insights. These nuclei serve as epistemic anchors rather than definitive explanations.

2. Narrative Envelopes

Concentric or peripheral interpretive layers that situate predictions within broader material, technological, and societal contexts, enabling integrative understanding across scales.

3. Connective Logics

Steering mechanisms—conceptual, ethical, and interpretive—that mediate transitions between prediction and narrative, preserving coherence while preventing epistemic drift.

Together, these elements define a fluid epistemic structure in which scientific reporting becomes an act of guided interpretation, prioritizing integration over isolation and reflexivity over accumulation. **Table 2** summarizes the core components of the proposed framework and their respective epistemic functions, risks, and steering mechanisms.

Table 2. Framework components, epistemic functions, and steering logics

Framework	Conceptual description	Primary epistemic	Key steering logic	Risk if unsteered
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component		function		
Predictive nuclei	Aggregated model outputs, uncertainty ranges, and learned correlations	Anchor interpretation in quantitative evidence	Scope signaling and uncertainty marking	Overconfidence and false finality
Narrative envelopes	Contextual layers (microstructure, application, sustainability, societal impact)	Enable systems-level sense-making	Selective emphasis and contextual balance	Narrative inflation or dilution of rigor
Connective logics	Interpretive rules linking predictions to narratives	Maintain coherence across epistemic layers	Recursive feedback and interpretive recalibration	Epistemic drift or incoherence
Epistemic boundary	Ethical and conceptual constraints surrounding interpretation	Prevent speculative overreach	Boundary articulation and transparency	Persuasive excess and misrepresentation
Feedback structures	Bidirectional loops between prediction and narrative	Support adaptive reinterpretation	Iterative refinement of priors	Static or self-reinforcing narratives

Figure 1 illustrates this framework: it depicts a central circular node labeled “Predictive Core” that represents aggregated properties.

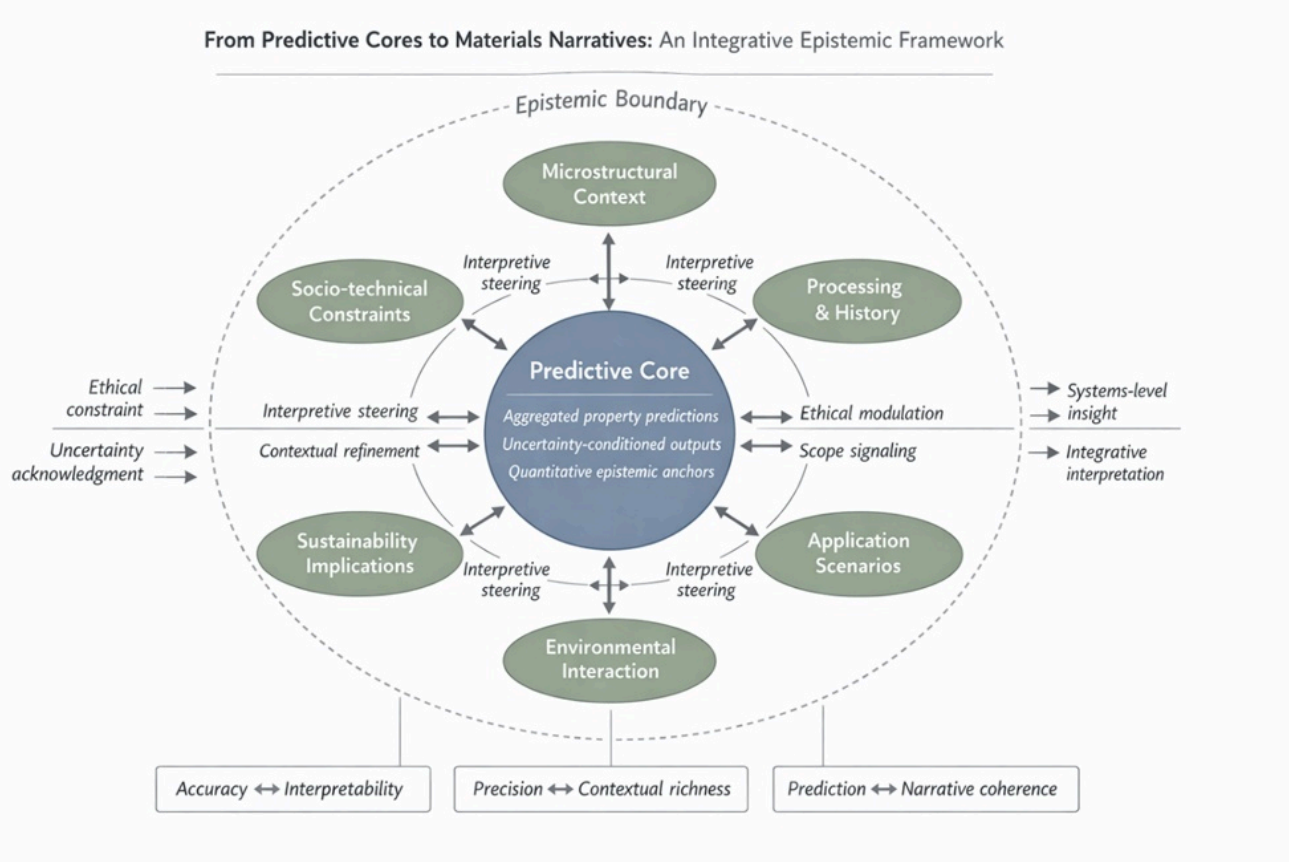


Figure 1. From predictive cores to materials narratives: an integrative epistemic framework

Through this lens, the framework offers conceptual tools for navigating the complexities of scientific reporting, where narratives emerge as interpretive scaffolds that enrich predictive foundations. Interaction dynamics emphasize the role of

steering mechanisms in maintaining coherence, while epistemic reasoning explores how such structures promote inclusive knowledge dissemination. Ultimately, the framework invites reflection on the broader interpretive potentials in materials discourse, prioritizing integrative over isolative approaches.

Analytical implications

The conceptual shift toward materials narratives carries profound analytical implications for the structuring and dissemination of knowledge in materials science. Interpretive dynamics at play reveal how narrative frameworks transform isolated predictive outputs into relational constructs, where properties are no longer viewed as standalone endpoints but as elements within evolving stories of material identity and function. This reconfiguration invites analysis of epistemic layering: predictive cores provide quantitative anchors, while narrative envelopes introduce contextual depth, creating a gradient of interpretive resolution that accommodates both precision and ambiguity [1, 3, 5].

One central implication concerns the modulation of uncertainty. In purely predictive paradigms, uncertainty is often treated as a residual to be minimized through model or dataset refinement. Narrative approaches, however, interpret uncertainty as an intrinsic feature of complex systems, incorporating it as thematic variability within the story arc—such as sensitivity to processing conditions or lifecycle degradation pathways. This interpretive stance does not diminish predictive value but reframes it, allowing uncertainty to become a productive element in systems-level understanding rather than an epistemic deficit [7, 9, 11].

Trade-offs in communicative efficacy constitute another analytical dimension. Narratives enhance accessibility and interdisciplinary resonance by employing relational language and thematic coherence, yet they introduce risks of selective emphasis or interpretive overreach. Steering logics within the framework—such as deliberate foregrounding of certain contextual layers over others—become critical mechanisms for navigating these tensions. The analytical insight here is that effective narrative construction requires explicit awareness of these steering choices, ensuring that integrative potential does not compromise scholarly restraint [6, 13, 15].

Feedback structures further illuminate dynamic implications. As predictive insights feed into narrative development and narratives in turn prompt reinterpretation of predictions, a recursive loop emerges that continuously refines conceptual coherence. This recursion supports adaptive knowledge production, where initial material characterizations evolve through successive narrative iterations, reflecting real-world complexities without requiring empirical revalidation at each step [12, 18, 21]. Systems-level analysis thus reveals narrative frameworks as self-correcting interpretive engines, capable of sustaining long-term epistemic evolution in rapidly advancing fields.

Ethical-analytical considerations also arise from the power asymmetry between predictive precision and narrative persuasion. Narratives can amplify the perceived significance of certain material attributes or applications, potentially influencing resource allocation or policy priorities in subtle but consequential ways. The framework's emphasis on epistemic boundary conditions—explicitly delineating where interpretation transitions into speculation—serves as an analytical safeguard, promoting reflective practice that interrogates the origins and limits of narrative authority [2, 4, 6].

Finally, the shift implies a reorientation of evaluative criteria in scientific reporting. Traditional metrics centered on predictive accuracy give way to hybrid standards that also assess narrative fidelity, thematic integrity, and integrative capacity. This expanded evaluative landscape encourages materials scientists to cultivate dual competencies: rigorous quantitative reasoning alongside sophisticated narrative craftsmanship [8, 10, 12]. The analytical outcome is a more pluralistic epistemology in which diverse modes of understanding coexist and mutually inform one another.

Results and Discussion

The interpretive transition from property prediction to materials narratives reflects deeper transformations in how scientific communities construct and share an understanding of matter. Rather than representing a rejection of computational

prediction, the shift constitutes an expansion of expressive repertoire, enabling the field to grapple with phenomena whose complexity exceeds the grasp of isolated quantitative statements.

Interaction dynamics between predictive and narrative modes reveal inherent complementarities. Predictive models excel at establishing causal anchors and bounding possibility spaces; narratives excel at situating those anchors within multidimensional contexts, revealing emergent patterns and relational dependencies that single-point predictions obscure [14, 16, 17]. This complementarity does not imply equivalence—predictive rigor remains foundational—but suggests that narrative elaboration functions as a necessary epistemic amplifier in domains characterized by multiscale coupling, environmental contingency, and application diversity.

Epistemic implications extend to knowledge circulation. Materials narratives, by virtue of their integrative structure, lower barriers to cross-domain comprehension. Concepts that once required specialized training are now accessible through well-crafted stories of material behavior, facilitating collaboration among chemists, engineers, physicists, environmental scientists, and even non-technical stakeholders [19, 20, 22]. Yet this democratizing potential is accompanied by responsibility: narrative clarity must not be achieved at the expense of conceptual precision. The framework's steering logics—selection of focal themes, calibration of interpretive scope, maintenance of traceable links to predictive nuclei—offer practical guidance for preserving scholarly standards amid increased communicative reach.

Another layer of discussion concerns temporality and narrative arc. Property prediction typically operates in a static, atemporal mode, delivering snapshot evaluations. Materials narratives introduce temporal dimensionality, tracing developmental trajectories from synthesis through service life to end-of-use. This temporal framing aligns scientific reporting more closely with lifecycle thinking prevalent in sustainability discourses, enabling richer conceptualizations of material responsibility and circularity [19–21]. The consequence is an expanded interpretive horizon that encompasses not only what a material is, but what it becomes across time and contexts.

Limits of the narrative paradigm must also be acknowledged. Excessive reliance on storytelling risks diluting quantitative nuance or introducing unintended anthropomorphic framing. The framework counters this by insisting on bidirectional feedback: narratives remain tethered to predictive cores, and predictive interpretations are continually tested against narrative coherence. This reciprocal constraint preserves analytical tension essential to scientific integrity [12, 19, 23].

In broader philosophical terms, the shift signals a move toward a post-representational epistemology in materials science—one that recognizes representation not as a mirror but as an active interpretive practice. By treating scientific reports as constructed narratives rather than neutral transcripts, the field aligns itself with constructivist insights already at work in other domains while retaining its commitment to empirical grounding through predictive validation [18, 22]. This alignment enriches disciplinary self-understanding without surrendering methodological discipline.

Conclusion

The conceptual movement from property prediction to materials narratives marks an evolutionary inflection in the epistemology of materials science. It does not supplant quantitative prediction but recontextualizes it within integrative interpretive structures that better capture the relational, contingent, and developmental character of matter.

Through this lens, scientific reporting becomes an act of narrative craftsmanship, where predictive insights serve as anchoring motifs within larger stories of material possibility, limitation, and transformation. The proposed framework—centered on predictive nuclei, narrative envelopes, connective logics, and epistemic boundaries—provides conceptual scaffolding for enacting this transition thoughtfully. Steering mechanisms ensure that integrative ambition remains disciplined, while feedback dynamics sustain ongoing refinement of understanding.

The implications reach beyond technical discourse. By embracing narrative modes, materials science enhances its capacity to engage societal questions of sustainability, equity, and responsible innovation. Narratives offer vehicles for

conveying not only what materials can do, but why their stewardship matters across ecological, economic, and cultural dimensions.

Ultimately, this shift invites the community to cultivate a dual fluency: mastery of predictive tools alongside sophistication in narrative construction. Such fluency promises more holistic, accessible, and ethically attuned scientific communication—capable of illuminating complex realities in ways fragmented predictions alone cannot. As materials science confronts multiscale challenges in an era of accelerating technological and environmental change, the narrative turn offers a vital interpretive resource for navigating uncertainty with clarity, coherence, and responsibility.

Acknowledgements

None

Conflict of interest

None

Financial support

None

Ethics statement

None

Received: 03 May 2022

Revised: 01 Jun 2022

Accepted: 11 Jul 2022

Published online: 18 January 2023

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